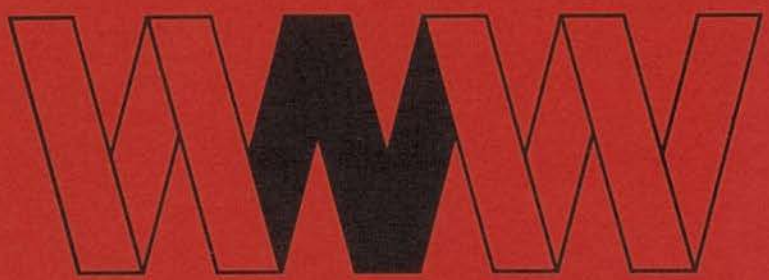
CONFERENTIE VAN NUMERIEK WISKUNDIGEN

29 september – 1 oktober 1986

CONFERENTIEOORD WOUDSCHOTEN
ZEIST



Werkgemeenschap Numerieke Wiskunde

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Werkgemeenschap Numerieke Wiskunde

Uitgave verzorgd door
CENTRUM VOOR WISKUNDE EN INFORMATICA TE AMSTERDAM

ELFDE CONFERENTIE NUMERIEKE WISKUNDE

Doel van de conferentie

De Conferentie Numerieke Wiskunde wordt eenmaal per jaar gehouden onder auspiciën van de Werkgemeenschap Numerieke Wiskunde. Het doel van de conferentie is om kennis te nemen van recente ontwikkelingen binnen de numerieke wiskunde. Hiertoe worden jaarlijks twee thema's vastgesteld. Lezingen over deze thema's worden normaliter verzorgd door uitgenodigde buitenlandse en binnenlandse deskundigen.

Thema's

1. *Numerieke roostergeneratie en adaptieve roosters*

2. *Stabiliteitstheorie in de numerieke oplossing van tijdsafhankelijke partiële differentiaalvergelijkingen*

Organisatie

De organisatie is in handen van de voorbereidingscommissie bestaande uit de heren Boerstoel (NLR) (voorzitter), Traas (THT), van der Vorst (THD) en Verwer (CWI) (secretaris), en van het Centrum voor Wiskunde en Informatica.

Uitgenodigde Sprekers

Thema 1. M.J. Baines, University of Reading, England
P.R. Eiseman, Columbia University, New York, USA
N.P. Weatherill, Aircraft Research Association LTD, Bedford, England

Thema 2. M. Crouzeix, Université de Rennes, France
J.M. Sanz-Serna, Universidad de Valladolid, Spain
J.C. Butcher, University of Auckland, New Zealand

Tijdens de laatste fase van de voorbereidingen heeft Prof. Thomée zich helaas wegens onvoorziene, drukke werkzaamheden moeten terugtrekken. De voorbereidingscommissie heeft in zijn plaats Prof. Butcher bereid gevonden als uitgenodigde spreker deel te nemen. Dit is mogelijk gebleken omdat hij vanwege een sabbatical in Europa verblijft. Wij willen onze erkentelijkheid uitspreken voor zijn bereidwilligheid om ondanks een zeer druk reisschema aan de Woudschoten Conferentie deel te nemen.

H.W.J. Lenferink (RUL), M.J. Officier (WL) en G.H. Schmidt (KSEPL) hebben zich aangemeld voor een korte voordracht.

Programma

Maandag 29 september

10.00-11.15	aankomst, koffie	15.15-15.45	thee
11.15-12.15	opening, Eiseman	15.45-16.45	Baines
12.30	lunch	16.45-17.15	Schmidt
14.15-15.15	Sanz-Serna	18.00	diner

Dinsdag 30 september

-8.00	ontbijt	12.45	lunch
-9.00-10.00	Butcher	14.15-15.15	Eiseman
10.00-10.30	koffie	15.15-15.45	thee
10.30-11.30	Weatherill	15.45-16.45	Sanz-Serna
11.30-12.30	Crouzeix	16.45-17.15	Lenferink
		18.00	diner

Woensdag 1 oktober

-8.00	ontbijt	12.45	lunch
-9.00-10.00	Baines	13.45-14.15	Officier
10.00-10.30	koffie	14.15-15.15	Butcher
10.30-11.30	Crouzeix	15.15	sluiting, thee, vertrek
11.30-12.30	Weatherill		

De bar is geopend van 17.00-18.00 uur en van 20.30-24.00 uur.

Titels en Samenvattingen Voordrachten

Maandag 29 september

11.15	opening P.R. Eiseman	*Numerical grid generation*
14.15	J.M. Sanz-Serna	*Nonlinear instability*
15.45	M.J. Baines	*The solution of evolutionary partial differential equations on self-adaptive grids by the moving finite element method*
16.45	G.H. Schmidt	*Adaptive local grid refinement and multigrid in numerical reservoir simulation*

Dinsdag 30 september

9.00	J.C. Butcher	*Stability and accuracy for initial value methods*
10.30	N.P. Weatherill	*Grid generation in computational aerodynamics*
11.30	M. Crouzeix	*Equivalence between A-stability and G-stability*
14.15	P.R. Eiseman	*Adaptive grids*
15.45	J.M. Sanz-Serna	*Nonlinear instability*
16.45	W. Lenferink	*Contractivity in the numerical solution of initial value problems by multistep methods*

Woensdag 1 oktober

9.00	M.J. Baines	*Applications of the moving finite element method to non-linear hyperbolic and parabolic problems*
10.30	M. Crouzeix	*On the discretization in time of semilinear parabolic equations with non smooth initial data*
11.30	N.P. Weatherill	*Block structured grid generation for aerodynamic geometries*
13.45	M.J. Officier	*Experience with numerical grid generation techniques and their application in flow problems*
14.15	J.C. Butcher	*Stability and accuracy for initial value methods*

THE SOLUTION OF EVOLUTIONARY PARTIAL DIFFERENTIAL EQUATIONS ON SELF-ADAPTIVE GRIDS BY THE MOVING FINITE ELEMENT METHOD

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In recent years there has been much interest in the use of adaptive grids in the solution of differential equation problems using both finite difference and finite element methods. One example of this approach is the Moving Finite Element method, introduced by Miller in 1981, in which the movement of the grid is computed automatically as the solution evolves in time. It will be shown that this approach gives rise to a local method in one dimension which gives the evolution of each linear segment of the solution independently. Generally the method has a structure which lends itself to rapid solution techniques and accurate resolution of special features, particularly moving fronts.

APPLICATIONS OF THE MOVING FINITE ELEMENT METHOD TO NON-LINEAR HYPERBOLIC AND PARABOLIC PROBLEMS

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In this talk we present applications of the Moving Finite Element method to a number of test problems. Key features are linear elements, a direct approach to parallelism and to node overtaking (avoiding penalty functions), rapid inversion of the mass matrix by pre-conditioned conjugent gradients and explicit Euler time stepping. Part of the talk will be devoted to a significant change of dependent variable which is of great assistance in numerical front tracking techniques for non-linear diffusion problems. Examples of the use of the method in both hyperbolic and parabolic problems will be given.

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STABILITY AND ACCURACY FOR INITIAL VALUE METHODS

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Introduction.

Although most high quality software for the solution of the initial value problem in ordinary differential equations is based on linear multistep methods, there is a strong body of theoretical evidence which would suggest that this is not necessarily the best choice. In these lectures, we will briefly survey the nature of this evidence especially in the light of the type of problem which arises from the method of lines.

The natural next choice, if linear multistep methods are to be avoided, is a method of Runge-Kutta type. There are severe difficulties in implementing these one-step methods in practice and some of these difficulties will be discussed. It is remarkable that the strengths of one type of method almost exactly coincide with the weaknesses of the other and it becomes appropriate to consider members of a wider class of method in the hope that useful compromises can be found between known methods where the worst disadvantages of each are avoided.

The wider class of methods that will be considered, constitutes "General Linear Methods" and the properties of these will be considered in some detail. In particular, it will be noted that many theoretical questions extend quite naturally to these new methods and that they do seem to have numerical properties which provide the expected compromise.

Pathological problems. What was at one time regarded as the standard problem type, $y'(x) = f(x, y(x))$, with f satisfying a Lipschitz condition with small Lipschitz constant and with the solution y a smoothly varying function, is now seen to be a poor representation of the variety of problems that arise in practice. Of course by "small" in the sense of Lipschitz constants we mean in terms of units which are natural to a physical problem being modelled. Thus, if L is the Lipschitz constant and h is a natural step-size in the direction of the independent variable in the sense that, after an interval h has elapsed, there will have occurred only a barely perceptible change in the solution, then we might wish to consider problems in which Lh is small compared with 1.

There are at least three important types of situations where this is not a useful assumption. The first is the situation that the problem being solved is stiff. In this case even though the natural step length is determined by a slowly varying smooth solution with any quickly decaying transients damped to an extent that they are invisible to practical measuring devices, they quickly reveal themselves through unstable behaviour when any

attempt is made to carry out a numerical computation based on the classical type of explicit method. Since the largest decay rates determine the Lipschitz constant, the difficulty of affecting a numerical solution is closely related with a high value of hL.

A second type of difficult problem is one in which the suppressed, but potentially dangerous, part of the solution coresponds not so much to rapid decay but to rapid oscillation. Again the value of hL is large and again computation by traditional explicit methods is not appropriate. In the third type of problem the behaviour of a physical system is described not simply by differential equations, but by a combination of differential and algebraic equations. Although this can be viewed as a limiting case of a stiff problem, it is now realised that it can present difficulties all of its own.

One of the most important types of stiff problem arises when a time dependant partial differential equation is discretized in the spatial directions using the method of lines. Stiffness is an intrinsic aspect of this approach as we can see by considering the spectrum of the linear operator in the finite dimensional discretized problem where we note that the operator which it approximates is unbounded. Elementary considerations based on the diffusion problem adequately illustrate this point.

The failure of explicit methods with stiff problems is a consequence of the difficulty of approximating $\exp(z)$, when z has large magnitude and negative real part, using as an approximation, one of the roots of an equation of the form

$$c_0(z)\,w^k + c_1(z)\,w^{k-1} + c_2(z)\,w^{k-2} + \ldots + c_k(z) = 0, \qquad (1)$$

where c_0 has the constant value1 and c_1, c_2, ... , c_k are polynomials. Although it is not necessary to obtain an accurate approximation, it is at least essential, if instability is to be avoided, that the approximation should have magnitude less than 1 when this property is satisfied by the exponential function itself. Only by allowing c_0 also to be a polynomial is there any hope of achieving an approximation of this quality. It is with implicit methods that such a factor is present. These considerations lead to the concept of A-stability and various closely related devices for studying the stability of methods intended for use with stiff problems.

Stability definitions. If the simple test problem $y'(x) = qy(x)$, where q is a possibly complex number, is solved numerically so that the solution is supposed to advance a distance h, then the exact solution is multiplied by $\exp(z)$ where $z = hq$ and the numerical solution represented computationally as a vector is multiplied by a matrix for which the characteristic polynomial is of the form of (1). An A-stable method is one in which the solution sequence is bounded for $\mathrm{Re}(z) \leq 0$. In the case of linear multistep methods, the polynomial coefficients in (1) are all of first degree and A-stability is directly related to the location of the zeros in relation to

the unit disc. In the case of Runge-Kutta methods, $k = 1$ but c_0 and c_1 can have arbitrary degree. It is known that A-stability is impossible for linear multistep methods for which the order of approximation is greater than 2 but that there is no such restriction in the case of Runge-Kutta methods.

We will also discuss closely related definitions for which the value of q is allowed to vary and where the differential equation is non-linear but for which stable behaviour of the exact solution is assured. These lead to the ideas of AN-stability as well as algebraic stability and the special nature of this last concept in the case of special method classes.

Limitations of linear multistep methods. As has already been pointed out, order of accuracy is limited to two for the case of A-stable linear multistep methods. It is possible to go beyond this by relaxing the stiff A-stability requirement and it is on methods with this type of generalized performance that most practical differential equation software relies. However, there seems to be no alternative but to accept an order restriction as a cost of reasonable stability properties. Other limitations of linear multistep methods are characteristic also of methods of this type designed for non-stiff problems such as costs involved with step-size changing.

Limitations of Runge-Kutta methods. Even though A-stability is available coupled with high order of accuracy for these methods, this is at the expense of abnormal implementation costs. Another difficulty is that the high order available with certain Runge-Kutta methods is not realisable in practice because of a deterioration of behaviour in the presence of stiffness when the "stage order" is much lower than the overall order. For these reasons, diagonally implicit and singly implicit methods have come under consideration. Other limitations characteristic of Runge-Kutta methods applied to either stiff or non-stiff problems are associated with the difficulty of obtaining inexpensive estimates of truncation error for step-size control purposes. Some progress will be reported on efforts to overcome thes limitations without leaving the general class of Runge-Kutta methods.

General linear methods. Although these have been known for many years as providing a unifying theory, practical prospects have only recently been explored. A survey will be presented of some of their properties and will emphasise ways in which they seem to overcome some of the difficulties inherent in other methods. Also some of their newly discovered stability properties will be discussed. It is hoped that there is time to present an outline of a proof that AN-stability is equivalent to algebraic stability for general linear methods. This generalizes known results for the special cases of one-leg methods and Runge-Kutta methods.

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EQUIVALENCE BETWEEN A-STABILITY AND G-STABILITY

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In order to solve the ordinary differential equation

$$y'(t) = f(t,y(t)) \quad , \quad t \geq t_0 \quad , \quad y(t_0) = y \quad ,$$

we consider the linear r-step method

$$\sum_{i=0}^{r} \alpha_i \, y_{n+i} = \Delta t \sum_{i=0}^{r} \beta_i \, f(t_{n+i}, y_{n+i}) \qquad , \qquad n \geq r-1 \, ,$$

or the corresponding one-leg method

$$\sum_{i=0}^{r} \alpha_i \, y_{n+i} = \Delta t \, f\Big(\sum_{i=0}^{r} \beta_i t_{n+i} \, , \sum_{i=0}^{r} \beta_i y_{n+i} \Big) \, ,$$

where Δt denotes the timestep and y_n an approximation of $y(t_n)$ at the time $t_n = n \Delta t$; we assume here that $\sum \beta_i = 1$.

These two schemes are caracterized by the two polynomials

$$\rho(\zeta) = \sum_{i=0}^{r} \alpha_i \, \zeta^i \quad , \quad \sigma(\zeta) = \sum_{i=0}^{r} \beta_i \, \zeta^i \quad .$$

According to G. Dahlquist, these schemes are A-stable when they satisfy the condition

$$\text{(A)} \qquad |z| \geq 1 \quad \Rightarrow \quad \mathrm{Re}\, \rho(z) \overline{\sigma(z)} \geq 0 \quad .$$

We prove that this condition is equivalent to

$$\text{(B)} \qquad \begin{cases} \text{There exist polynomials } p_1, \ldots, p_r \, , q \, , \\ \text{with } d^\circ p_j \leq r-1 \text{ and } d^\circ q \leq r \, , \text{ such that} \\ \rho(z)\sigma(w) + \rho(w)\sigma(z) + (1 - zw) \sum_j p_j(z) \, p_j(w) = q(z) \, q(w). \end{cases}$$

Furthermore, if ρ and σ have no common factor , the polynomials p_j are lineary independant .

Then, we use (B) to reobtain the results of G. Dahlquist :

" An A-stable method has an order less than or equal to two ",

and

" A-stability is equivalent to G-stability ".

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ON THE DISCRETIZATION IN TIME OF SEMILINEAR PARABOLIC EQUATIONS WITH NON SMOOTH INITIAL DATA

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We shall begin by recalling some results concerning the discretization in time of the linear homogeneous equation

(1) $\quad u_t + Au = 0 \quad \text{for} \quad t > 0, \; u_t = \frac{\partial u}{\partial t}$,

where A is a self-adjoint positive definite operator in a Hilbert space H (cf., e.g., BAKER, BRAMBLE and THOMEE [1]).

Let r(z) be a rational function having no poles for $z \geq 0$, and define an approximate solution U_n at $t = t_n = nk$, where k is the time step, by

$$U_{n+1} = r(kA)\, U_n \quad \text{for } n = 0,1,2,\ldots,$$
$$U_o = v.$$

Assume that the approximation is of order p with $p \geq 1$, or

(2) $\quad r(z) = e^{-z} + O(z^{p+1})$ as $z \to 0$,

and also that the method is stable in the sense that

$$|r(z)| \leq 1 \quad \text{for} \quad z \geq 0.$$

Then one may show the "smooth data" error estimate

$$\|U_n - u(t_n)\| \leq C\, k^p\, \|A^p v\| \quad \text{for } v \in D(A^p).$$

This follows easily from spectral representations and the fact that under our assumptions

$$|r(z)^n - e^{-nz}| \leq C\, z^p \quad \text{for } z \geq 0.$$

In applications the requirement $v \in D(A^p)$ is quite restrictive. For example, if A is an elliptic partial differential operator in a domain $\Omega \subset R^d$, it demands not only smoothness of the initial data but also that they satisfy certain compatibility conditions at the boundary $\partial\Omega$ for $t = 0$. However, under the stronger stability assumption

(3) $$|r(z)| < 1 \quad \text{for} \quad z > 0, \text{ and } |r(\infty)| < 1,$$

one can also show the "non-smooth" data error estimate

(4) $$\|U_n - u(t_n)\| \leq C\, k^p\, t_n^{-p}\, \|v\| \quad \text{for } v \in H,\ t_n > 0.$$

This follows again by spectral arguments from

$$|r(z)^n - e^{-nz}| \leq C\, n^{-p} \quad \text{for} \quad z \geq 0,$$

and shows that even with v only in H, the $O(k^p)$ convergence is retained for $t_n > 0$. It follows also that for $0 \leq q \leq p$ the intermediate estimates

(5) $$\|U_n - u(t_n)\| \leq C\, k^p\, t_n^{-q}\, \|A^{p-q} v\| \quad \text{for} \quad v \in D(A^{p-q})$$

hold.

The question we want to address below is to what extent these error estimates with reduced regularity assumptions carry over to semilinear equations. Thus assume that $f(t,u)$ is a smooth function on $\overline{J} \times H$, where $J = (0,T]$ with $T < \infty$, and consider the semilinear problem

(6) $$\begin{aligned} u_t + Au &= f(t,u) \quad \text{for} \quad t \in J, \\ u(0) &= v\ . \end{aligned}$$

For its approximate solution we will investigate single-step discretization schemes of the form

$$U_{n+1} = r(kA)\, U_n + k\, F(k,t_n,U_n) \quad \text{for} \quad t_n \in \overline{J},$$

$$U_0 = v,$$

where $r(z)$ satisfies (2) with $p = 1$ and $F(k,t,v)$ is chosen to be consistent with (6) in a sense to be made precise below. As an example of such schemes, consider the standard first-order backward Euler scheme defined by

$$U_{n+1} = (I+kA)^{-1} U_n + k(I+kA)^{-1} f(t_{n+1},U_{n+1}), \tag{7}$$

or the linearized version

$$U_{n+1} = (I+kA)^{-1} U_n + k(I+kA)^{-1} f(t_n,U_n), \tag{8}$$

where in the first case $F(k,t_n,U_n)$ is defined implicitly by (7). We shall be able to show that for such schemes

$$\|U_n - u(t_n)\| \leq C\, k\, t_n^{-1} \operatorname{Log} \frac{t_{n+1}}{k} \quad \text{for} \quad t_n \in J,$$

where C depends on an upper bound for $\|v\|$, so that for first-order schemes the estimate (4) essentially remains valid in the semilinear case.

We shall then demonstrate that, more surprisingly, it is not in general possible to generalize the higher order estimate (4) with $p > 1$ to semilinear equations. This will be done by exhibiting a simple system of the form (6) such that, for any choice of a Runge-Kutta method satisfying (3), and any $t \in J$, we have

$$\limsup_{n=t/k\to\infty} \|U_n - u(t_n)\| \geq c\, k \quad \text{with} \quad c = c(t) > 0.$$

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The two primary categories for numerical grid generation are algebraic methods and partial differential equation methods. In distinction, algebraic methods come from explicit algebraic formulas while partial differential equation methods come implicitly from the equations as solutions. Both contain conformal mapping as part of their historical roots but both have progressed in a distinctly more general direction to address the more arbitrary constraints arising from practical situations. To satisfy the constraints, the element of control over the transformations has become the most important aspect. Control can be exercised in a fixed, programmed manner, in a dynamic interactive session, and in an adaptive context. In the general applications setting, the transformations are generated with varying degrees of automation and are assembled to form grids with topologies that conform best to the given physical problems. The topological issues are typically done in a multi-block format and will be addressed by Weatherill in his lectures. The present lecture will therefore emphasize the aspects of control in a single transformation.

The fundamentals of algebraic grid generation consist of first establishing the general class of unidirectional transformations and then establishing the general framework for assembling the directions. The unidirectional transformations come from multisurface transformations and the assembly comes from transfinite processes. The discussion starts with the development of the general multisurface transformation and then proceeds to the special cases. These include the classical shearing and cubic Hermite transformations (sometimes called the "two-boundary techique"), the piecewise polynomial forms for

local controls,and also a piecewise trigonometric form for the same purpose but with a simpler defining statement.

To maintain generality in the transfinite assembly of directions, we return to the arbitrary multisurface transformation which contains the various special cases. The first assembly operation is that of a tensor product which conforms to an array of control points but not to the full boundaries of prescribed regions. By itself this operation involves finitely many data points and thus is not transfinite. The tensor product transformation can be decomposed into steps which progressively operate in increasing dimensions starting with the control points themselves. With just the points in each direction, each coordinate-wise sequence can be used to define a corresponding curve directly from the multisurface transformation. Treating sequences of such control curves in the same manner as the control points, we obtain the tensor product transformation for two dimensions or a sequence of control surfaces in three dimensions. An application of the multisurface transformation to the control surfaces yields the three-dimensional tensor produce transformation. In these constructions, the order in which directions are taken is unimportant.

The next fundamental operation is the creation of a Boolean sum of multisurface transformations. In each direction, the multisurface transformation is based upon fully defined control curves or surfaces that altogether form an intersecting network. Rather than assuming that such a network is supplied as input, we shall consider the simpler special case where the boundaries together with an array of control points are supplied. With this assumption, the construction of intermediate control curves or surfaces is the same as in the tensor product case. Together with the boundaries, multisurface constructions are then established for each direction. On a given boundary in two dimen-

sions, the construction using that boundary reproduces it while the transverse construction produces a curve that also comes from the tensor product construction. By subtracting the tensor product from the regular sum we obtain precisely the given boundary. This operation is called the Boolean sum and the result is transfinite since an entire boundary with generally an infinite number of points is fit. The applications in three dimensions follow the same pattern and are straightforward. The double sum produces a fit to all boundaries of a distorted cube. In each dimension, a somewhat sparse array of internal control points is available for the manipulation of the grid within the boundaries.

In the other category of methods, the grid is the numerical solution to a system of partial differential equations. Here, the controls are determined by the system definition. Of the various types of defining systems, those which are elliptic contain the strongest control properties; albeit, they are not as fast as the hyperbolic and parabolic methods that can generate grids in one marching pass through a region. The speed issue is somewhat tempered, however, by the availability of fast numerical algorithms and fast computers. As a consequence, the ability to control the outcome is the primary concern; and thus, we focus our attention upon elliptic partial differential equations which are more simply called "elliptic methods." We start by considering the Laplace system of Winslow and then progress into the Poisson system of Thompson, Thames, and Mastin where controlling terms are first inserted. To understand the basic controls in the simplest possible manner, we examine their construction and effect first in one dimension and then in higher dimensions. Next, the various ways in which the controls are applied is examined. This includes the inward propagation of boundary distributions, the specification of angles and spacing at boundaries, and the utilization of curvature.

In continuation, a natural framework to view elliptic methods is provided by variational statements. In such statements, the controls are easily established for distinct purposes, but the actual execution is much more complex.

To conclude our discussion, we examine some pre- and post-processing strategies. The first concerns the creation of pointwise distributions on curves where precise numbers of points can be clustered in various regions, where endpoint spacing can be prescribed and where a uniform level of curvature clustering can be applied. This is followed by the post-processing strategy of inserting local clusters into arbitrary grids and then by the assembly of grids by means of a partition of unity.

ADAPTIVE GRIDS

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Adaptive grids have become necessary when significant solution variations appear on finer length scales than can be provided by a fixed grid. This situation typically occurs when the variations appear with unknown strength and position and are evolving in time. To provide the required resolution, a mechanism to monitor the evolution of the variations must be established and then employed to drive the grid points into the correct positions. The driving motion occurs when the grid generation controls are activated by the monitored quantities. Altogether, the grid point motion must appear as an automatic response to a changed solution. When coupled with a scheme to advance the solution in time, we have an adaptive grid simulation. While similar simulations can be done by locally altering the number of grid points, we note that the basic well-ordered nature of a grid is depreciated by producing internal boundaries that require special treatment. As a consequence, we will restrict our attention to only those situations where motion is the primary mechanism. Dynamic changes in the number of points will then only be considered on a global basis.

To start our discussion, we will establish a "monitor surface" as a means to consolidate the adaptive data into one simply defined object that can be reliably used to monitor the evolution of rapid variations in a solution. While solutions commonly appear as vector quantities, we shall strive to define such monitor surfaces with only a scalar quantity at each point in physical space. This represents a real simplication since the surface is then embedded in a Eulidian space of only one dimension higher.

With the assumption of a monitor surface, we may then proceed to consider

grid generation methods that are sufficiently reliable and automatic to provide the desired motion while retaining a decent grid structure. These methods can be developed in either of two natural ways: either the basic grid generation is performed on the surface or it is done in physical space. If the generation occurs directly on the surface, then the physical space grid is just the downward projection of the surface grid. The advantage of the surface grid generation is that a uniform grid there automatically resolves the gradients in physical space. As a consequence, the demands upon weight functions are light. In contrast, the basic grid generation in physical space is simpler but the demands upon weight functions are heavier.

Regardless of the location where the grid generation is performed, the basic constructive principles remain the same. Moreover, virtually all of the basic methods have roots in the one-dimensional setting. In that context, we can then understand the basic elements without undue mathematical detail. As a consequence, we are drawn to consider the process in which a weight function is to be equally distributed between the successive points of a grid on a curve. This process is then varied and interpreted from a number of viewpoints and in various distinctive forms.

With a basic understanding established, we next proceed to consider higher dimensions. The most direct extension into higher dimensions is to apply adaptivity on a curve by curve basis and to cycle through one or more coordinate directions. The methods of this description are called "alternating direction adaptive methods." From a geometric viewpoint, these methods operate by specifying the diagonal part of the metric tensor since each such entry is inversely proportional to a specified weight. With the weights, metric relationships are enforced, various clustering quantities are employed, and prescribed distributions are inserted. Among the clustering quantities are the

magnitudes of gradients and the various forms of curvature (e.g., normal, geodesic, and mean).

While the straight curve by curve adaptation yields good results in many circumstances, there is a significant underlying limitation on the weights. Namely, the weights cannot be too severe or else the procedure will collapse. This has been observed and while corrective action can be inserted directly into the process, such action is rather detailed and technical.

It has recently been found that a better course of action is to redefine the directional sweeps by splitting them into two phases: the active phase and the passive phase. In the active phase we just have our original curve by curve strategy in the current direction. This contains the fundamental adaptive forces. In the passive phase, a "low pass filter" is applied to remove any wiggles or abrupt changes in spacing caused by the active phase but to leave intact the basic results of the intended action. This produces a smooth grid in the sense of derivative continuity. As a consequence, continuous numerical derivatives are available for numerical solution algorithms and for the application of controls in successive sweeps. Such controls include the use of orthogonality and curvature in the weights. As a practical matter, it has been observed that the splitting of sweeps into this predictor-corrector format of active and passive phases has resulted in considerably enhanced stability and a much larger range of severity in the choice of weights.

Also in a recent study, the curve by curve weights that specify the diagonal part of the metric tensor have been inserted into the popular Poisson equation format where curvilinear variables are dependent variables. The consequence is that the grid evolves smoothly as in the case with the prior passive phase. In distinction, here, the measure of smoothness is a closeness to conformal conditions as opposed to the direct previous measure of derivative

continuity. This can be seen in the various grids. Quite simply, the conformal conditions being stronger more rapidly cut off the adaptive action. As a result, the more distant grid points are barely moved by the adaptive motion. In a further note of comparison, the Poisson format is substantially slower in a computational sense, but is more easily set up in a general topological situation. The application of the alternating direction approach to general grid topologies simply requires some special treatment.

With the basics firmly established by considering cases that evolved by applying controls along coordinate curves, we next consider methods based upon cell volumes and integral statements. These methods follow the established pattern of objectives and have their own distinctive characteristics. The methods that we will consider include mean value relaxation and variational methods. In addition, we will also consider general connectivity triangular meshes.

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CONTRACTIVITY IN THE NUMERICAL SOLUTION OF INITIAL VALUE PROBLEMS BY MULTISTEP METHODS

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Let $\|.\|$ be an arbitrary norm on $\mathbb{R}^s$. Consider the initial value problem in $\mathbb{R}^s$

$$(1) \qquad \begin{cases} U'(t) = A(t)U(t) , & t \geq 0 \\ U(0) = u_0 , \end{cases}$$

where the real s×s matrix A(t) satisfies a circle condition $\|A(t) + \rho I\| \leq \rho$ for $t \geq 0$, some $\rho > 0$. The exact solution of (1) is dissipative, i.e. $\|U(t_2)\| \leq \|U(t_1)\|$ for all $t_2 \geq t_1 \geq 0$.

To guarantee a numerical analogue of this property when solving (1) by a multistep method, the stepsize h should satisfy a restriction of the form $h \leq R\rho^{-1}$, where R depends only on the method.

For the class of linear k-step methods of order p there exists an optimal value R(k,p) for R. Properties of R(k,p) and the corresponding methods will be given.

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EXPERIENCE WITH NUMERICAL GRID GENERATION TECHNIQUES AND THEIR APPLICATION IN FLOW PROBLEMS

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In this presentation we want to give a survey of the grid-generation techniques that are presently available at the DHL. The use of these methods in two of our standard computer-programs will be presented, both in the theoretical formulations and some applications.
As techmiques we describe two algebraic methods, one non-orthogonal elliptic method, an orthogonal elliptic method with prescription of the local griddensity and finally the use of a digitizer as generator.
The use of one of the mentioned methods in an adaptive way for a problem with moving internal boundaries will be given.
For our problems we have some special wishes like: local contraction of the gridlines, near-to-orthogonality constraints for boundary-conditions, ease of adaption of the domain with respect to future obstacles like breakwaters in a harbour lay-out. The numerical methods of calculating the grids are given.
The two mentioned standard computer-programs are described in some detail and the consequences of the transformations both for the involved discretizations and interfacing problems are shown.
To illustrate the above mentioned, six applications in both shallow-water calculations and two-dimensional Navier-Stokes equations are presented.
This presentation is essentially based upon a paper presented at The First International Conference on NUMERICAL GRID GENERATION IN COMPUTATIONAL FLUID DYNAMICS in last July in Landshut.

NONLINEAR INSTABILITY

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First Talk

It is well known that, in politics, many widely different forms of government call themselves *democratic*. In a like manner, numerical analysts use the word *stability* in a large number of non-equivalent senses. Correspondingly, the expression *nonlinear instability* can be understood in many ways. Very loosely speaking, we employ the word instability whenever we find situations where something *goes wrong*. An instability is *nonlinear* when things go wrong with a nonlinear algorithm, in spite of the fact that some sort of *linear* analysis has predicted that things should be all right. (By linear analysis we mean here an analysis based on replacing the nonlinear discretization being investigated by a linear approximation thereof.)

In the first talk we shall be more *specific* in the use of the word *instability* and we shall only employ it to refer to cases where the discretization of an evolutionary problem results in a numerical solution with *unbounded growth*, while the theoretical solution itself remains bounded for all times. Linear constant coefficient examples of such an unwanted growth are easily provided: when applied to the ODE $du/dt = iu$, (u complex), the convergent Euler rule generates growing solutions, regardless of the choice of time step τ. Some features of this and similar linear growths are: (i) They are felt right from the first time-steps. (ii) They occur regardless of the particular initial condition being used. (iii) They are exponential. (iv) They can easily be predicted analytically by studying the discrete equations.

Due to the fourth property above, this form of linear growth can

be avoided in practice, at least in constant coefficient cases. In nonlinear situations, an analysis of the discrete equations is often difficult, and one must therefore resort to what we called above a linear analysis. Phillips was the first person to report (1959) that nonlinear algorithms, stable according to linear analyses, can lead to growth (nonlinear instability). This growth: (i) Often needs many time-steps before it is felt. (ii) Depends on the initial condition. (iii) It can be more violent than exponential. (iv) It is difficult to analyze.

The work of Phillips was followed, among others, by Richtmyer & Morton (see Section 5.6 of their book) and Stetter (1966) with Fornberg (1973) giving the most transparent example. In the talk we shall survey a number of examples of nonlinear instability in PDEs. These case-studies can be divided into two groups: (a) Cases where the growth is due to the space discretization. Here we will deal with Fornberg's $u_t+uu_x = 0$ example and more recent material relating to the Burgers equation (Aref & Daripa (1984), Eastwood & Arter (1986)). (b) Cases where the growth is due to the time-stepping. Here we will mainly follow the speaker's work with Vadillo.

The issue of how to avoid offending growths will be addressed next, with the focus on: (i) Spatial discretizations with conservation properties (Arakawa's schemes (1966); Galerkin discretizations, see Morton (1977)). (ii) Recent advances in nonlinear investigations of time-stepping schemes (see Dekker & Verwer (1984) for a survey).

Finally we will critically assess the effectivity of the suggested cures of the nonlinear instability phenomenon.

Second talk

The first talk has limited itself to unphysical growth, one of the forms of pathological behaviour that can be present in a linearly stable nonlinear algorithm. We shall present next other possible pathologies including (i) trouble with solving the discrete equations in implicit discretizations and (ii) chaos (Ushiki (1982), Mitchell & Griffiths (1986), Prüfer (1985)).

Of importance is the fact that all the nasty behaviours described so far can be present in commonly employed, useful schemes. Thus the question arises of how to bring together the *pathologies* that can turn up in practice and the notion of *convergence*. In the remainder of the talk we shall address the question of how to define a notion of *Lax-stability* for nonlinear discretizations. A successful definition should satisfy (at least) the following conditions: (i) It should be strong enough to imply, together with consistency, the existence and convergence of the numerical solutions. (ii) It should not be so strong as to classify as unstable algorithms currently being employed with success. (iii) It should be general enough to cater for most classes of problems found in practice. (iv) It should not be so general and abstract that it becomes of no use when facing a given, concrete example.

A definition will be presented that, in our opinion, successfully meets the four requirements above. The talk here will mainly follow material by López-Marcos and the speaker, but the underlying ideas can be traced back to Stetter (1966) and Keller (1975). The key feature is that stable nonlinear algorithms exhibit a threshold effect: they show insensitivity to perturbations *provided that these are small enough*. The fact that we adequately allow for such a threshold effect enables us to prove a neat equivalence result: A (smooth) nonlinear discretization is stable according to the suggested definition if and only if its linearly stable.

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ADAPTIVE LOCAL GRID REFINEMENT AND MULTIGRID IN NUMERICAL RESERVOIR SIMULATION

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Abstract:

Flexible gridding has the potential of increasing the accuracy in numerical simulation of flow through hydrocarbon reservoirs within limitations in computing time and memory space. The adaptive gridding method presented here follows general concepts outlined by Brandt. The pressure equation is discretised on locally refined grids with mixed finite elements. A multi-grid solution method is stated for the (indefinite) set of equations in the pressure and its gradient (or flow). A proof of convergence of the multi-grid process is given and convergence rates are discussed. The method has been tested on a set of equations representative for reservoir simulation. Results obtained for a five-spot example are shown.

Keywords:

Dynamic local grid refinement, mixed finite elements, multi-grid, multi-phase flow, numerical reservoir simulation.

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GRID GENERATION IN COMPUTATIONAL AERODYNAMICS

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Many problems in the physical sciences and engineering involve the numerical solution of a set of equations in a complicated shaped domain. The solution of such problems requires the domain to be discretised to produce a set of points on which the numerical algorithm can be based. For some problems, the generation of a suitable grid is as demanding as the effort required to perform the computations for which the grid was intended. In recent times, considerable attention has been focused on the discretisation process, which is commonly called grid generation. The proceedings of two conferences devoted to grid generation provide a good outline of techniques used for different scientific and engineering applications (1,2).

In the last fifteen years, computational methods have played an ever increasing role in the field of aerodynamic design. The Full Potential, Euler and more recently, time-averaged Navier-Stokes equations have been used to model the air flow over aerodynamic shapes. The technical difficulties associated with the numerical solution of these equations are considerable. However, grid generation for aerodynamic shapes has not progressed as rapidly as flow algorithm development and today the development of suitable techniques for the discretisation of the flow field around complicated aerodynamic shapes is recognised as a pacing item in computational aerodynamics. Examples of complicated configurations include multi-element aerofoils in two dimensions and any geometry more complex than a wing-body combination in three dimensions.

The common goal of different grid generation techniques is to construct boundary fitted coordinates which enable the solution of the field equations

in domains of arbitrary shape. Grid generation is technically difficult since it is not sufficient, in most applications, to arbitrarily define the position of points. It is intuitively obvious that the greater the number of points in the computational grid, the more accurate the numerical solution. However, computer memory and execution times restrict the number of points. Grid generation is thus an optimisation problem; given a finite number of points, how can a flow field be best resolved? The choice of a curvilinear coordinate system can have a substantial effect on the error in the numerical solution of a partial differential equation. It is essential to ensure that grid point clustering occurs in the regions where the gradients in the unknown variables are large so as to capture the main details of the physics embodied within the governing equations. The truncation error introduced into the numerical procedure is dependent not only on higher order derivatives of the variables and local grid spacing but also on the rate of change of grid spacing and departure of the grid from orthogonality.

From these comments, it may seem relevant to ask what are the quantitative requirements for a good grid. A knowledge of limits on grid skewness, cell aspect ratio, grid point stretching would be of considerable value. However, the science of flow algorithm sensitivity to grid properties is not well developed and the quality of a grid is invariably judged by eye. In grid generation for aerodynamic shapes, it is also inappropriate to question whether a given distribution of points for a geometry is the ultimate most efficient grid for that particular shape. All too frequently, the generation of an acceptable grid is an achievement in itself. Only recently has the literature reported the automatic generation of a grid around a complete transport aircraft (3,4).

In the early development of computational aerodynamics, conformal mapping techniques were used. The classical method of conformal grid generation is to map a contour (an aerofoil, engine inlet etc) to a circle by a single or sequence of simple transformations and then to define a network of r = constant, θ = constant lines. When such mappings are inverted, the resulting orthogonal grid in physical space provides a suitable set of points at which to solve the flow equations. An example of this approach to two-dimensional multi-element geometries has been given by Grossman and Volpe (5). As the geometrical complexity of the configuration increases, so the requirement for more sophisticated mappings grows. In addition, conformal techniques do not readily generalise to grid generation in three dimensions. These restrictions have led to the development of other techniques.

The equations used to generate grids do not have to possess any physical significance. This aspect has been fully exploited and grid generation equations of elliptic, parabolic and hyperbolic type have been investigated.

One of the major grid generation techniques now in use is to determine grid point coordinates by the solution of a system of elliptic partial differential equations. This approach can be traced to Winslow (6) but has been made popular by Thompson, Thames and Mastin (7). In this method, Laplace's equation is used as the generating system, ie

$$\xi_{xx} + \xi_{yy} = 0 \qquad (1)$$

$$\eta_{xx} + \eta_{yy} = 0$$

where (ξ,η) and (x,y) are the computational and physical coordinates respectively. Since it is appropriate to perform the numerical computation in a rectangular transformed plane, it is necessary to interchange the dependent and independent variables in eq (1). The equations then obtained are

$$\alpha\, x_{\xi\xi} - 2\beta x_{\xi\eta} + \gamma x_{\eta\eta} = 0$$

$$\alpha\, y_{\xi\xi} - 2\beta y_{\xi\eta} + \gamma y_{\eta\eta} = 0$$

where the metric terms are

$$\alpha = \left(\frac{\partial x}{\partial \xi}\right)^2 + \left(\frac{\partial y}{\partial \xi}\right)^2, \quad \beta = \frac{\partial x}{\partial \xi} \cdot \frac{\partial x}{\partial \eta} + \frac{\partial y}{\partial \xi} \cdot \frac{\partial y}{\partial \eta}, \quad \gamma = \left(\frac{\partial x}{\partial \eta}\right)^2 + \left(\frac{\partial y}{\partial \eta}\right)^2.$$

These equations readily generalise to three dimensions and have been used by a number of researchers (8,9,10).

Grid generation using parabolic and hyperbolic equations has not been as popular as technqiues based on elliptic equations. The nature of parabolic and hyperbolic equations restricts their use to particular geometries in which the grid can be marched away from a relatively simple boundary shape. Their application in aerodynamics has been confined to bodies or space shuttle configurations (11,12).

In most grid generation problems points are known on several or all the boundaries of the computational domain and the problem consists of extending these boundaries into the interior of the domain. Perhaps the simplest solution to this problem is direct linear interpolation of the boundary points to the interior. More complex forms of interpolation have been developed and all are referred to as algebraic methods. The multisurface method of Eiseman (13) and transfinite interpolation (14,15) have both proved successful technqiues.

The grid generation techniques already discussed produce, in two dimensions, a set of quadrilateral cells which lead to a high degree of structure in the mesh. Each point has the same number of neighbours and the relationship between points can be readily described by direct addressing within a computer memory. For multiply connected regions such as the domain around a multi-element aerofoil and for complicated three dimension regions, for example, near a nacelle/pylon/wing, the structure imposed by rows and columns of quadrilateral/hexahedral cells can become very restrictive. The subdivision of the flow domain into blocks, where the arrangement of the blocks allows grid structures local to each component to be defined, goes some way to alleviate the problem (8). This so-called multiblock grid generation will be the subject of the second lecture. It can be argued that the quadrilateral shape is not the best unit with which to break down a complicated region. For complex geometrical domains, it may seem more appropriate to use the lowest order topological simplex, namely the triangle in two dimensions and the tetrahedron in three dimensions. In fact, finite element techniques have been traditionally based on these simple shapes.

A new, unstructured triangular grid generation procedure for aerodynamic shapes has recently been developed (4,16). The method uses the concept first described by Dirichlet in 1850, whereby a given domain can be systematically decomposed into a set of pack convex polygons. Given a set of points in the plane, the Dirichlet tessellation is the construct which assigns to each point a territory that is the area of the plane closer to that point than to any other point in the set. If the set of points is denoted by $\{p_i\}$, then the Dirichlet region $\{D_i\}$ can be defined as

$$D_i = \{p : ||p - p_i|| < ||p - p_j||, \forall_j \neq i\} .$$

The sum of all the points p forms a Dirichlet polygon or Voronoi region. The territorial boundary which forms the side of a Dirichlet polygon is midway between the two points which it separates and is thus a segment of the perpendicular besector of the line joining these two points. If all point pairs which have a segment in common are joined by straight lines, the result is a triangulation of the convex hull of data points. This triangulation is known as the Delaunay triangulation. These ideas extend to three dimensions.

Using the concept of the Dirichlet tessellation and its dual, the Delaunay triangulation, a grid around a complicated geometry can be constructed. Sets of grid points appropriate to particular regions or components are defined by

any appropriate technique (conformal mapping, elliptic, algebraic etc). The points from all sets are then connected using the Dirichlet concept. This method has been exploited in two dimensions for multiply connected domains (16) and in three dimensions for a complete aircraft geometry (4).

The technqiues briefly described above will be discussed in the lecture. Examples will be given for aerodynamic geometries but the ideas are applicable to other fields of numerical computation.

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BLOCK STRUCTURED GRID GENERATION FOR AERODYNAMIC GEOMETRIES

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In the first lecture, 'Grid Generation in Computational Aerodynamics', an overview was presented of grid generation techniques. In the second lecture, it is proposed that a method based on the elliptic equations, which is applicable in two and three dimensions, and which has been successfully applied to a wide range of aerodynamic geometries, will be described (1-4).

The rapid advance in computer technology, coupled with improved flow algorithms, has brought the possibility of flow simulation for realistic aircraft configurations much nearer to fruition. However, to date, most flow simulations have been restricted to relatively simple configurations, such as wing/body combinations, because of the difficulty of generating grids around more complex configurations. Most of the production codes now widely in use in industry are based on ad hoc grid generation procedures, such as conformal mapping coupled with stacked two-dimensional grids (5). While such procedures have proven valuable in producing high quality grids for a restricted range of problems, their inherent limitations suggest an alternative, more flexible approach is necessary for general aircraft geometries.

It is now generally recognised that the fundamental problem associated with grid generation for general configurations is that each component in the configuration (wing, body etc) has its own natural type of grid topology (such as an O or C grid for wing, O grid for a body etc) but that these topologies are usually incompatible with each other. This has led to the idea of generating grids whose topology is locally consistent with each component but with some global means of connecting the grids. Such approaches are usually described as multiblock or zonal or composite grid approaches because the complete flow region is broken down into blocks or zones local to each component.

The mechanism by which the regions are connected leads to a variety of approaches. Atta and Vadyak (6) generate the local component grids completely independently and use overlapping of the grids together with interpolation of the flow variables to transfer information between grids. Alternatively, Lee (7) divides the flow region into a set of blocks and generates the grids essentially independently in each block subject to the constraint that grid lines meet point for point at the block boundaries. This approach leads to grids which may be non-smooth at these boundaries. Recently, other approaches have been described which utilise the multiblock concept (8,9,10).

The approach to be described in the lecture is similar in concept to that of Lee (8) in that the flow region is divided into a series of blocks chosen to match the general topology of the configuration and to give grid structure most appropriate for each component. However, the grids are not generated independently in each block, instead they are generated simultaneously in all blocks using an elliptic grid generator.

Central to our multiblock approach is the idea that the whole flow field between the surfaces of the configuration and some outer far-field boundary is conceptually broken down into a set of blocks. The union of these blocks fills the entire flowfield without either holes or overlaps. Each block is chosen to be topologically equivalent to a cuboid in that it has six faces and eight corners and can, therefore, in principle, be mapped into a unit cube in computational space without change in topological structure. Cartesian grids in the unit cubes in computational space map back to curvilinear grids in physical space.

The procedure used to perform the mapping is the elliptic grid generation approach of Thompson, Thames and Mastin (11). In this approach, the coordinates (x,y,z) defining the grid nodes in physical space are obtained as the solution of non-linear elliptic partial differential equations in which the independent variables are the computational coordinates in the unit cubes. In the grid generation, some block faces represent parts of the configuration surface or parts of the outer boundary. On such faces, which are referred to as Dirichlet faces, the grid distribution is calculated by a surface grid generation procedure. Other faces represent the junction of two blocks and as such are purely notional boundaries which, provided the grid lines pass smoothly through the junction, have no physical significance. On such boundaries, which are called continuity boundaries, the grid generation equations are solved at each point as though

the points were inside the block since program logic is used to access the coordinates of points in neighbouring blocks required in the solution procedure. Hence, the grid is as smooth at these boundary points as at any point inside a block.

The information needed to define the block structure and the interrelationship between blocks is supplied to the system by the user in a 'topology file'. This consists of a list of all faces of all blocks giving, for each face, the type of boundary conditions for the grid generation and flow calculations and, where appropriate, the adjacent block number, face number and orientation of the adjacent face relative to the current face. Eight possible orientations of one face relative to another can be defined but only four of these are topologically valid for any particular pair of faces.

Given a suitable topology structure for a given geometry, the multiblock system consists of four components. A geometry package, tailored to the grid generation approach, which has a component intersection capability and is based on bi-cubic surface patches (12), transforms each component surface into parametric coordinates $S = (s,t)$. The generation of the grids on the surface of the configuration is then performed in terms of these parametric coordinates. The grid points are generated from the elliptic equation (11) in which the dependent variables are (s,t). Having obtained the distribution of (s,t) on each component, the grid points are mapped back to physical space via the bi-cubic patch data. A similar approach is used to generate grids on the outer farfield boundary. Once the boundaries of the flow domain have been discretised, the necessary boundary conditions are available to solve for the grid points in the field. Again, the elliptic equations are used. On completion of the field grid calculation, the resulting set of grid points is used with an algorithm to solve the Euler equations and which is based on the ideas of Jameson, Schmidt and Turkel (13) which has been structured to accept multiblock grids.

In order to ensure good grid quality, ie suitable grid point clustering, low cell skewness and acceptable cell aspect ratios, the elliptic equations are augmented with source terms. The source functions are computed from the technqiue described by Thomas and Middlecoff (14). The elliptic equations are solved using block-by-block iterative routines which include an approximate factorisation and a successive over-relaxation point technique.

The lecture will describe in greater detail, the multiblock concept and the grid generation solution procedure. Examples of grid structures on a variety of aerodynamic configurations will be given.

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