CONFERENTIE VAN NUMERIEK WISKUNDIGEN

15, 16 en 17 oktober 1984

CONFERENTIEOORD WOUDSCHOTEN
ZEIST

Werkgemeenschap Numerieke Wiskunde

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Uitgave verzorgd door
CENTRUM VOOR WISKUNDE EN INFORMATICA TE AMSTERDAM

NEGENDE 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 deskundigen.

THEMA'S

De thema's zijn:

1. *De numerieke oplossing van evolutieproblemen met toepassingen op Navier-Stokes- en Eulervergelijkingen.*
2. *Iteratieve methoden voor niet-symmetrische stelsels van lineaire algebraïsche vergelijkingen.*

ORGANISATIE

De organisatie is in handen van de voorbereidingscommissie bestaande uit de heren Axelsson (KUN), Boerstoel (NLR), van Veldhuizen (VU) en Verwer (CWI), en van het Centrum voor Wiskunde en Informatica.

UITGENODIGDE SPREKERS

Thema 1. J.J. Chattot, Matra Industries, Velizy
B. van Leer, Technische Hogeschool Delft
H. Viviand, ONERA, Parijs

Thema 2. R. Beauwens, Vrije Universiteit Brussel
J. Periaux, Avions Marcel Dassault, Parijs
D.M. Young, University of Texas, Austin
G. Golub, Stanford University (onder voorbehoud)

De Heer Chattot komt in de plaats van Temam. Op het gebied van de Euler-vergelijkingen werkt hij samen met de groep van Prof. Temam.

Tijdens de laatste fase van de voorbereidingen is gebleken dat Prof. Golub rond half oktober zal deelnemen aan een conferentie in Leuven. Dit was voor de organisatiecommissie aanleiding hem uit te nodigen ook een voordracht in Zeist te verzorgen (binnen thema 2).

A.O.H. Axelsson en H. Schippers hebben zich aangemeld voor een korte bijdrage.

PROGRAMMA

Maandag 15 oktober

10.00-11.15	aankomst en koffie	15.15-15.45	thee
11.15-12.30	opening, Young	15.45-16.45	Periaux
12.45	lunch	16.45-17.15	Schippers
14.15-15.15	van Leer	18.00	diner

Dinsdag 16 oktober

8.00	ontbijt	12.45	lunch
9.00-10.00	Viviand	14.15-15.15	Periaux
10.00-10.30	koffie	15.15-15.45	thee
10.30-11.30	Beauwens	15.45-16.45	van Leer
11.30-12.30	Chattot	16.45-17.15	Axelsson
		18.00	diner

Woensdag 17 oktober

8.00	ontbijt	12.45	lunch
9.00-10.00	Chattot	13.45-14.45	Golub(onder voorbehoud)
10.00-10.30	koffie	14.45-15.45	Young
10.30-11.30	Viviand	15.45	sluiting,thee, vertrek
11.30-12.30	Beauwens		

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

TITELS EN SAMENVATTINGEN VOORDRACHTEN
(De samenvattingen van Chattot en Periaux zijn niet in dit programma opgenomen. Indien beschikbaar zullen deze aan het begin van de conferentie worden uitgereikt)

Maandag 15 oktober

11.15	opening	
	D.M. Young	*Introduction to Iterative Algorithms for Solving Nonsymmetric Linear Systems*
14.15	B. van Leer	*Conservative Dissipative Difference Schemes for Hyperbolic Equations*
15.45	J. Periaux	*Domain Decomposition Least Squares and Conjugate Gradient Methods applied to Nonlinear Problems in Fluid Dynamics*
16.45	H. Schippers	*Numerical Integration of the Unsteady Full-Potential Equation with Applications to Transonic Flow about a 2D-Airfoil*

Dinsdag 16 oktober

9.00	H. Viviand	*A Multi-Domain Matching Technique for Hyperbolic Systems. Application to Inviscid Euler Flow Calculation*
10.30	R. Beauwens	*Description of OBV Factorization Algorithms*
11.30	J.J. Chattot	*On Euler and Navier Stokes Differential Equations*
14.15	J. Periaux	*Domain Decomposition Least Squares and Conjugate Gradient Methods applied to Nonlinear Problems in Fluid Dynamics*
15.45	B. van Leer	*The Numerical Representation of Discontinuities in Weak Solutions*
16.45	A.O.H. Axelsson	*On Preconditioning Methods for Convection-Diffusion Problems*

Woensdag 17 oktober

9.00	J.J. Chattot	*On Euler and Navier Stokes Differential Equations*
10.30	H. Viviand	*Navier-Stokes Flow Calculation Using a Multi-Domain Approach and a Zonal Mesh Refinement Technique*
11.30	R. Beauwens	*Analysis of OBV Iterative Methods*
13.45	G. Golub	
14.45	D.M. Young	*Iterative Algorithms and Software for Solving Large Sparse Nonsymmetric Linear Systems*

On preconditioning methods for convection-diffusion problems

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Recently new types of incomplete factorization methods based on sparse matrix approximations of the inverses of diagonal block matrices have been developed. It has been proven that such methods exists for an arbitrary M-matrix.

We survey some methods of the above type and discuss how they can be used in connection with the more general matrix problems one encounters for convection dominated convection-diffusion problems.

I. DESCRIPTION OF OBV FACTORIZATION ALGORITHMS

II. ANALYSIS OF OBV ITERATIVE METHODS

(extended abstracts)

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I. DESCRIPTION OF OBV FACTORIZATION ALGORITHMS

1. Introduction

Factorization iterative methods were introduced around 1960 but remained almost unnoticed until the numerical investigations of Stone in 1968. They received much attention during the last decade, being twice rediscovered and more than twice generalized to sparse block factorization iterative schemes. The large number of different versions and results which came out justifies the search for a synthetic approach. It is the purpose of the present talk to define an approach called "OBV formalism" covering most of these methods and reasonably suitable for their theoretical analysis.

A basic ingredient of this formalism is the use of the Hadamard multiplication, denoted $A * B$, of matrices $A = (a_{ij})$ and $B = (b_{ij})$ of the same dimensions, defined by

$$(A * B)_{ij} = a_{ij} b_{ij} \quad .$$

We observe here that the Hadamard multiplication by a (0,1) matrix, i.e. a matrix whose entries are equal to zero or unity, provides a convenient mathematical notation for the masking operation, so commonly used to define iterative methods.

2. Background

We consider the solution of the linear system $Ax = b$ where A is an $n \times n$ real or complex matrix by iterative schemes of the first order, i.e. of the form

$$Bx_{m+1} = Cx_m + b \qquad (2.1)$$

where x_m denotes the successive iterates and $A = B - C$; alternatively (2.1) may be written

$$B(x_{m+1}-x_m) = b - Ax_m \quad . \tag{2.2}$$

By definition, we call it a (block) factorization iterative method when equation (2.1) or (2.2) is solved via (block) LU-factorization of B.

It may of course be accelerated; polynomial relaxation and multigrid techniques have been used for this purpose.

3. The OBV formalism

We assume that A is partitioned into submatrices A_{ij} of dimensions $n_i \times n_j$, i,j=1,2...m and that the vectors x and b are similarly partitioned into block components X_i and B_i of dimensions n_i, i=1,2...m. For reference purpose, this partitioning is denoted by π and the matrices and vectors so partitioned are termed π-partitioned vectors and matrices. We use the notation $diag_\pi(A)$ to denote the block diagonal π-partitioned matrix with block diagonal equal to that of A. When m = n, π is called the point or p-partitioning and $diag_p(A)$ is more simply written diag(A).

We further write the LU-factorization of B under the form $B = LP^{-1}U$ where L and U are lower and upper block triangular π-partitioned matrices and P is block diagonal, together with the normalization condition $diag_\pi(L) = diag_\pi(U) = P$.

The essential step in the definition of a factorization method is to relate the approximate factors L,P and U to the given matrix A. In the following, we call (block) OBV methods those (block) factorization methods for which there exists n x n (π-partitioned) matrices α and β of scalar parameters (called iteration parameters) such that

$$L + U - P = \alpha * A - \beta * ((L-P)K(U-P)) \tag{3.1}$$

where K is a block diagonal π-partitioned matrix (representing an approximation to P^{-1}). We stress that α and β may but need not be given beforehand.

4. Classification

One merit of the OBV formalism is to give some guiding lines to classify the litterature, distinguishing between truly new methods and new types of relaxation techniques (that could have been termed generalized SSOR and USOR methods). The classification so suggested will be used in this section to briefly review the litterature. We also take this opportunity to briefly mention implementation considerations.

5. Existence analysis

Factorization algorithms may fail; this happens for the block OBV factorizations when some block component of P turns to be singular; although this occurence need not prevent us from executing the approximate factorization itself, it does prevent us from being able to solve Eq. (2.1) or (2.2) with respect to x_{m+1}. It is therefore desirable to determine conditions under which OBV methods will not fail. Such conditions will be reviewed in this section.

It is worth to mention that some of these results define iteration parameters conjectured as close to the best ones when using polynomially accelerated OBV methods.

II. ANALYSIS OF OBV ITERATIVE METHODS

1. Introduction

In this talk, we attempt to review the proven and conjectured convergence properties of OBV iterative schemes.

Two approaches have been considered. The first one rests on the theory of regular splittings. It allows an intercomparison between point and block OBV methods. Methods of this class have been recommended as smoothers for multigrid techniques.

In the second case, we consider the OBV factorization strategies to be recommended for polynomially accelerated OBV methods. A challenging conjecture is formulated and proven results are reviewed.

We conclude with implementation considerations.

2. Convergence analysis

Convergence and comparison theorems that have been obtained by applying the theory of regular splittings will be reviewed in the present section. In these investigations, the matrix A is assumed to belong to the class of M-matrices or of H-matrices or to some generalization of these classes of matrices. On the other hand, some restrictions are put on the admissible range for the iteration parameters (i.e. the entries of the matrices α and β). The methods covered in these investigations include a.o. those used as smoothers for multigrid techniques.

3. Comparison between point and block schemes

The comparison theorems reviewed in Section 2 allow intercomparisons between block methods associated with one and the same partitioning. On the other hand, given some block OBV factorization of A associated with some partitioning, say π , and given some subpartitioning π' of π, it is possible to determine a block OBV method associated with π' and giving rise to the same splitting matrix B.

As a consequence, it is possible to compare point and block methods of similar complexity and to show that, when applied to M-matrices, block factorization schemes are faster than corresponding point factorization schemes.

4. Factorization strategies for polynomially accelerated OBV methods

A nice perturbation technique was introduced by Axelsson and further developed by Gustafsson to prove that, when applied to Stieltjes matrices, factorization iterative schemes are able, under appropriate conditions, to reach a convergence rate larger by an order of magnitude than that of classical schemes. Gustafsson observed however that the perturbations introduced to prove this result seemed actually unnecessary to reach it in practice. An alternate (and algebraic) approach was developed by the present author, bringing partial confirmations of the conjecture of Gustafsson. On the other hand, Axelsson and Gustafsson extended their technique to other classes of matrices including higher order finite element matrices and unsymmetric matrices.

An important practical issue of these investigations is that factorization strategies may be defined that are conjectured (and sometimes proved) as close to the optimal ones. A challenging mathematical problem is to prove it in the general case. Briefly stated, the rule to follow is to choose the OBV iteration parameters so as to realize $Ax = Bx$ (or $Ax = Bx$ + perturbing terms) where x is some appropriate positive vector. The same rule was found to play an essential role in existence analysis.

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Conservative Dissipative Difference Schemes for Hyperbolic Equations

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In solving problems of gas dynamics it is often permitted to ignore the dissipative processes in the gas, that is, viscous friction and heat conduction. This simplification of the physical picture boils down, mathematically, to a degeneration of the partial differential equations from second-order conservation laws, the Navier-Stokes equations, to first-order conservation laws, the equations of ideal compressible flow (ICF). Even in this approximation there remains a bewildering variety of complicated flow problems.

Particularly notorious are the problems involving such a strong compression of the gas that, in spite of the a priori assumption, dissipation sooner or later dominates the flow, at last in certain regions known as shocks. In a shock the flow quantities undergo a significant change over a distance typical of the dissipative interaction, i.e. the molecular mean free path.

It is, of course, impossible to infer the *structure* of a shock from the equations of ICF. The concept of ICF traditionally is saved and extended by representing a shock as a flow *discontinuity*.

The motion of such an idealized shock may be derived from an integral version of the first-order conservation laws, expressing the particular conservation principle for a finite volume of fluid and a finite lapse of time. Mathematically, this leads to the theory of weak solutions of nonlinear conservation equations. The algebraic equations relating the propagation speed of a discontinuity to its amplitude are called the jump equations.

Weak solutions are not unique. Shock discontinuities in which friction *produces* kinetic energy instead of dissipating it, and heat flows from lower to higher temparatures, are as eligible as their physically realizable counterparts. Clearly a selection criterion must be invoked. We shall accept a weak solution of the first-order conservation equations only if it is the limit solution, for vanishingly small dissipation, of the second-order conservation equations. For gasdynamics this is equivalent to the following requirement: the entropy of the gas, measure of the accumulated effect of dissipation, must not decrease in a shock. This is called the entropy inequality.

Thus, the advantage of lowering the order of the flow equations is partly offset by the need to introduce extra equations and an extra inequality. In consequence, analytic treatment of ICF problems is impossible in all but a few cases. The numerical treatment, however, can be entirely successful. The key to success is the combination of conservation and artificial dissipation.

The idea behind artificial dissipation is that, since in ICF the effect of dissipation is ignored, it may as well be *exaggerated.* By providing a difference scheme for ICF with sufficiently large dissipative terms it is possible to achieve that shocks, whenever these appear, posses a structure coarse enough to be resolved in the computational grid.

The concept of conservation enters if we make the difference scheme consistent with the integral form, rather than the differential form, of the equations of ICF. The scheme is then said to be 'conservative' or to have the 'conservation form'; another often-heard description is 'finite-volume scheme'. It has been shown, in theory and practice, that, in using a conservative scheme, the numerical stability of a solution containing an admissible shock automatically guarantees the correct motion of the shock. But in order to achieve numerical stability and to select the proper shocks, the scheme indeed has to be dissipative.

The Numerical Representation of Discontinuities in Weak Solutions

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Shock discontinuities, arising in weak solutions of initial-value problems based on hyperbolic conservation laws, are preferably treated with the aid of dissipative, conservative difference schemes. The numerical dissipation comes in the place of the disregarded physical dissipation, rendering stability and irreversibility to the numerical laws, valid across a shock.

Numerical dissipation can be added explicitly, as in the original artificial-viscosity method, or may be bidden in the difference equations, showing in a Fourier analysis or in an expansion of the truncation error. In the past decade, dissipation for higher-order schemes has often been implemented in the form of a switch between the higher-order and a first-order scheme (Harten, 1978), or a limiter of higher-order terms (Boris and Book, 1973; Van Leer, 1974).

A local lack of dissipation in a numerical shock profile can be recognized by post-shock and/or pre-shock oscillations. Monotony of the numerical solution therefore is the criterion by excellence in administering numerical dissipation (Van Leer, 1973). In fact, for any scheme, optimum expressions for dissipation coefficients, switches and limiters may be derived from the following principle:

The initial-value distribution that is assumed in between the nodal points shall have no more extrema than the set of nodal values.

Schemes for which this principle is easily implemented are the upwind finite-volume schemes of Van Leer (1979) and the diagonalizable conservative schemes of Roe (1981a). The former because, in each cell, explicit initial values are prescribed that can freely be manipulated; in the latter because these are as easy to handle as a scalar convection scheme.

Other schemes, while subject to the same principle, are less conveniently 'monotonized', unless these allow reformulation in the fashion of Roe.

Both upwind finite-volume schemes and diagonalizable conservative schemes require the use of an algorithm that solves, exactly or approximately, Riemann's intial-value problem, i.e. resolves an arbitrary discontinuity. Recent efforts have uncovered four entirely different, new algorithms with properties desirable for the application in difference schemes. These are

- the weighted-wave approximation of Harten and Lax (1981), designed for use in a random-choice method;
- the linear approximation of Roe (1981b);
- the simple-wave decomposition of Osher and Solomon (1982);
- the Boltzmann approximation (flux-vector splitting) of Van Leer (1982).

The most striking property of these 'approximate Riemann solvers' is the ability to render a stationary shock profile with no more than one (Harten and Lax, Roe) or two (Osher and Solomon, Van Leer) internal states. This forms a sound basis for post-process shock fitting.

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NUMERICAL INTEGRATION OF THE UNSTEADY FULL-POTENTIAL EQUATION WITH APPLICATIONS TO TRANSONIC FLOW ABOUT A 2D AIRFOIL

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The design of transonic-cruise transport aircraft requires the computation of unsteady airloads on oscillatory wings for application in flutter analysis. Flutter and other unsteady phenomena cannot be adequately predicted by extrapolating results of unsteady subsonic aerodynamic theory into the supercritical transonic flow regime. Instead, computational methods must be based on unsteady transonic aerodynamic theory to account properly for shockwave development and excursions. This motivates the development of algorithms for the accurate integration of unsteady transonic flow equations.

During the last decade, progress has been made in the numerical integration of the potential transonic small disturbance equation. For low-frequency motions, a fully implicit algorithm has been developed by Ballhaus and Steger [1]. The resulting code LTRAN2 has been extensively used despite its various limitations and has been at the basis of several 2D as well as 3D further extensions. For the calculation of airloads on thick blunt-nosed airfoils (e.g. supercritical airfoils) the transonic small disturbance formulation is less suitable. Here an improved approximation of the inviscid transonic flow problem is required. The best set of equations is then obviously the Euler equations. However, solving these equations is rather expensive in terms of computer time on the current generation of sequential high speed computers.
A substantial reduction of computer time can be achieved by assuming isentropic potential flow instead. In its most condense form this formulation results in the scalar second order full potential equation.

The integration in time of the unsteady full-potential equation is hampered by its non-linearity. In order to overcome this difficulty the equation is linearized about the flow field at a slightly earlier time-level.
The linearization process is carried through upto second order accuracy and results in a linear second order hyperbolic differential equation, which is integrated in time by an implicit splitting scheme of first order accuracy. This scheme is a modification of the fractional step method of Konovalov [2], which has been selected because of computational aspects and the stability property to be unconditionally stable for the 2-dimensional wave equation. However, in unsteady transonic potential flow computations it appears that the size of the time step is restricted because the truncation errors, introduced by the time-linearization process, become significant.

The full-potential equation is discretized in space by a fully-conservative finite-volume technique utilizing the concept of mass-flux splitting [3,4]. This concept replaces the usual artificial viscosity or artificial density concept and leads to improved non-linear stability properties. At sonic lines, expansion shocks are rigorously suppressed by applying an Engquist-Osher type switch whereas at shock points a Godunov type scheme is employed.

Numerical results are presented for unsteady transonic flow about a NACA 64A010 airfoil and an ONERA-M6 airfoil, undergoing sinusoidal pitching oscillations about the quarter chord position.

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A MULTI-DOMAIN APPROACH FOR THE COMPUTATION OF INVISCID OR VISCOUS FLOWS

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INTRODUCTION

A large variety of numerical schemes exists for the solution ofsystems of partial differential equations governing inviscid or viscous flows, and progress is continuing at a rapid pace in the field of numerical analysis especially for fluid mechanics. However, as more and more complicated flow problems are considered for numerical treatment, the increasing computing cost severely conflicts with the accuracy, so that much attention is now paid to the problem of optimal implementation of numerical schemes.

Three factors are determinant for the computing cost :

i) choice of mathematical model describing the flow (including the choice of the dependent variables),

ii) numerical algorithm used to solve this mathematical model,

iii) mesh size, or number of mesh points.

The factors i) and ii) are linked together since the choice of a mathematical model, although primarily dictated by its suitability to describe the physics of the problem, can also be influenced by the efficiency of existing schemes for this model.

It has long since been recognized that, for realistic flow problems, a unique choice for each of these three factors over the entire flow will not be optimum. Different flow regions, each one having its own physical characteristics, co-exist in a real flow and, in particular, length scales can vary by orders of magnitude from one region to another : inviscid flow region, shock wave, attached boundary-layer, free shear-layer, separation or reattachment regions, vortices, neighborhood of geometrical singularities (apex, corner, trailing-edge, wing tip...), shock-boundary layer interaction, etc.

It is clear, in view of the complexity of real flows, that much could be gained in computing cost if one were able in each region to use the mathematical model, the numerical algorithm and the mesh best suited and most economical for this region. This is the basis for the multi-domain or zonal approach which is not new but is now attracting more and more attention. This approach allows in principle to make the best choice of factors i) ii) and iii) for each region independently of the others. However the counterpart of this advantage is the need to provide each region with appropriate boundary conditions. Some of these conditions may be part of the boundary conditions associated with the complete flow field, but other boundary conditions will be required to express the matching of the solutions in adjacent regions. The matching problem is the key problem for the multi-domain approach, and it can be looked at in many different ways.

We present a study carried out at the Aerodynamics Department of ONERA on a general matching technique based on the use of compatibility relations for hyperbolic systems. This technique applies to time-dependent methods, the equations solved being hyperbolic with respect to time, at least in the vicinity of the matching boundary.

In the first part of this presentation, the general principles of the matching technique are discussed. In the second part, we present the application to the computation of inviscid flows (based on the Euler equations) and of viscous flows (based on the Navier-Stokes equations). For the latter case, we also emphasize a zonal mesh refinement technique used in the viscous layers.

The work presented here is the result of contributions by L. Cambier, W. Ghazzi, J.P. Veuillot and H. Viviand. More detailed presentations of various aspects of this work can be found in Refs. [1] to [5] .

Part I

A Multi-Domain Matching Technique for Hyperbolic Systems

1 - GENERAL PRINCIPLE -

Consider the following quasi-linear first order system of partial differential equations written in matrix form :

$$\frac{\partial f}{\partial t} + A_j \frac{\partial f}{\partial x_j} = 0 \qquad (1.1)$$

where f is the vector of the M scalar unknowns f_1 , f_2 , ... f_M , t is the time and x_j (j = 1, 2, 3 for 3D flows) are the space coordinates ; A_j are M x M matrices, known functions of f.

System (1.1) is supposed to be hyperbolic with respect to time ; it can be the full system of the Euler equations, or it can be some pseudo-unsteady formulation of steady equations governing iso-energetic flows or iso-energetic and homentropic flows (see Refs. [6] to [8] for detailed discussions of such pseudo-unsteady formulations).

We recall that for any unit vector $\vec{\nu}$ of space, there correspond M real eigenvalues $\lambda^{(k)}(\vec{\nu})$ and M linearly independent left eigenvectors $\alpha^{(k)}(\vec{\nu})$ such that :

$$\alpha^{(k)} \cdot \left(E(\vec{\nu}) - \lambda^{(k)} I \right) = 0 \qquad (1.2)$$

$$\det \left\{ E(\vec{\nu}) - \lambda^{(k)} I \right\} = 0 \qquad (1.3)$$

where the matrix E is given by

$$E(\vec{\nu}) = \sum_j \nu_j A_j \qquad (1.4)$$

By multiplying system (1.1) on the left by each eigenvector $\alpha^{(k)}$, for given ν, one obtains a system of linear combinations of the equations of (1.1) called compatibility relations (hereafter abbreviated as C.R.), completely equivalent to the original system (1.1) :

$$\alpha^{(k)} \cdot \left(\frac{\partial f}{\partial t} + A_j \frac{\partial f}{\partial x_j} \right) = 0 \qquad (1.5)$$

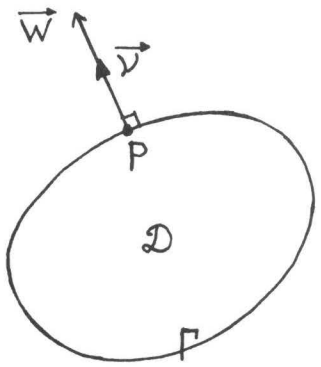
Taking into account Eq. (1.2), it can be shown that the C.R. (1.5) can be put into the form :

$$\alpha^{(k)} \cdot \left(\frac{\partial f}{\partial t} + \lambda^{(k)} \frac{\partial f}{\partial \nu} \right) = \alpha^{(k)} \cdot g \qquad (1.6)$$

where $\partial f / \partial \nu = \vec{\nu} . \mathrm{grad} f$ is the derivative of f in the direction of $\vec{\nu}$, and where g is a linear combination of derivatives of f only in directions normal to $\vec{\nu}$.

Thus the left-hand side of (1.6) is a combination of transport terms for each component of f, in the same direction $\vec{\nu}$ and with the same speed $\lambda^{(k)}$, whereas the right-hand side involves only derivatives of f in directions normal to $\vec{\nu}$.

Consider now the boundary Γ of domain $\mathcal{D}$ in which system (1.1) is to be solved. Let $\vec{\nu}$ be the unit outward normal at point P on Γ ; the boundary can move with the normal velocity $\vec{W} = W \vec{\nu}$. At point P we can write system (1.1) in the form of the C.R. (1.6) associated to the vector $\vec{\nu}$. We see, from the physical interpretation of (1.6) in terms of propagation of information in the direction $\vec{\nu}$ with speed $\lambda^{(k)}$, that a C.R. can be used at P only if it is physically meaningful, i.e. if it expresses a transport of information (relative to Γ) from the domain $\mathcal{D}$ or its boundary Γ to the point P, that is to say only if we have :



Notation for boundary treatment

$$\lambda^{(k)}(\vec{\nu}) - W \geq 0 \qquad (1.7)$$

Let us order the eigenvalues in such a way that $\lambda^{(k)}$ is a non-decreasing function of k, and assume that there are m eigenvalues strictly smaller than W ; so we can write :

$$\lambda^{(1)} \leqslant \lambda^{(2)} \leqslant \dots \leqslant \lambda^{(m)} < W \leqslant \lambda^{(m+1)} \leqslant \lambda^{(m+2)} \leqslant \dots \leqslant \lambda^{(M)} \qquad (1.8)$$

We deduce that the determination of f at the boundary point P should be based on :

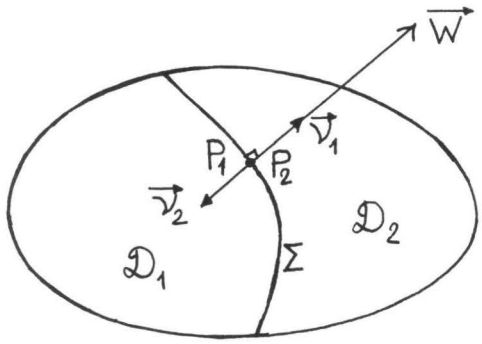
a) the (M - m) C.R. associated to $\vec{\nu}$ and to the eigenvalues $\lambda^{(k)}$ with $m + 1 \leqslant k \leqslant M$.

b) m boundary conditions to replace the m "missing" C.R.

This is the basis for the general method of treatment of boundary points used in Refs. [1] to [5] .

2 - APPLICATION TO THE MATCHING OF ADJACENT SUB-DOMAINS -

In the multi-domain approach, the solutions in two adjacent sub-domains $\mathcal{D}_1$ and $\mathcal{D}_2$ are coupled together through the boundary treatment to be applied at the common boundary Σ (also called hereafter interface) separating the two subdomains. This boundary treatment results simply from the application on Σ , and separately to each subdomain, of the general principle stated in section 1.



Notation for adjacent sub-domains

In the implementation of this principle, a point P on Σ splits into two points P_1 and P_2 depending on the sub-domain considered ; we shall call $\vec{\nu}_1$ the unit normal on Σ directed from $\mathcal{D}_1$ in $\mathcal{D}_2$, and $\vec{\nu}_2 = -\vec{\nu}_1$ the opposite normal. The speed of Σ at P is also written $\vec{W} = W_1 \vec{\nu}_1 = W_2 \vec{\nu}_2$, with $W_2 = -W_1$.

We shall distinguish also two cases depending on whether Σ is just an artificial interface (then f is continuous across Σ) or Σ is a physical discontinuity surface (shock wave or slip surface) (then f takes on different values on the two sides of Σ).

Then, applying the general principle stated in section 1, for subdomain $\mathcal{D}_1$, at P_1, we use the $(M - m_1)$ C.R. associated to the eigenvalues $\lambda_1^{(k)} = \lambda(\vec{\nu}_1, f(P_1), k)$, ordered as in (1.8), which verify :

$$\lambda_1^{(k)} - W_1 \gtrless 0 \tag{2.1}$$

and for subdomain $\mathcal{D}_2$, at P_2, we use the $(M - m_2)$ C.R. associated to the eigenvalues $\lambda_2^{(k)} = \lambda(\vec{\nu}_2, f(P_2), k)$, ordered as in (1.8), which verify :

$$\lambda_2^{(k)} - W_2 \gtrless 0 \tag{2.2}$$

In total, let $(2M - m)$ be the number of independent C.R. which apply at point P ; we then need m additional relations so as to be able to determine the 2M unknowns at P which are the components of $f(P_1)$ and $f(P_2)$.

In the first case when Σ is an artificial interface, with given speed W_1, we have the M continuity relations :

$$f(P_1) = f(P_2) \tag{2.3}$$

Then, and since $\vec{\nu}_2 = -\vec{\nu}_1$, we get :

$$\lambda_2^{(k)} = \lambda(\vec{\nu}_2, f(P_2), k) = \lambda(-\vec{\nu}_1, f(P_1), k) = -\lambda_1^{(M-k+1)} \tag{2.4}$$

Assume first that $\lambda_1^{(m_1+1)} \neq W_1$; then the relation (2.4) implies $m_1 + m_2 = M$ and $m = M = m_1 + m_2$. The m additional relations are just the M continuity relations (2.3).

Assume now $W_1 = \lambda_1^{(m_1+1)} = \ldots = \lambda_1^{(m_1+r)}$ which is so an eigenvalue of order r ($r \geq 1$) for $\mathcal{D}_1$; then the relation (2.4) implies $m_2 = M - m_1 - r$, and $W_2 = \lambda_2^{(m_2+1)} = \ldots = \lambda_2^{(m_2+r)}$ is an r-order eigenvalue for $\mathcal{D}_2$. Then the total number of C.R. to be used at P appears to be equal to $M - m_1 + M - m_2 = M + r$, so that there would be r extraneous relations. In fact, this is not so because the two sets of r C.R. which correspond to the r-order eigenvalue W_1 at P_1, and to the r-order eigenvalue W_2 at P_2 are identical ; this can be seen from (1.6) : $\partial/\partial t + W_1 \partial/\partial \nu_1 = \partial/\partial t + W_2 \partial/\partial \nu_2$ is simply the time-derivative at the point P moving with Σ, and the continuity of g and of $\alpha^{(k)}$ across Σ results from that of f.

In the second case when Σ is a physical discontinuity surface, the normal velocity W_1 of Σ is an additional unknown and we need $(m + 1)$ additional relations.

Assume first that Σ is a K-shock, which means, following Lax [9], that there exists an integer K such that :

$$\left.\begin{aligned} \lambda_1^{(K-1)} < W_1 < \lambda_1^{(K)} \\ \lambda_2^{(M-K)} < W_2 < \lambda_2^{(M-K+1)} \end{aligned}\right\} \tag{2.5}$$

We deduce

$$m_1 = K-1 \quad , \quad m_2 = M-K \tag{2.6}$$

The C.R. used on the two sides of Σ are independent, hence $m = m_1 + m_2 = M - 1$; the $(m + 1) = M$ additional relations are the jump relations (i.e. the usual Rankine-Hugoniot relations if system (1.1) is the full system of the Euler equations).

Assume now that Σ is a K-contact discontinuity, in which case [9] there exists an integrer K such that :

$$\left.\begin{aligned} \lambda_1^{(K)} = \lambda_1^{(K+1)} = \cdots = \lambda_1^{(K+r-1)} &= W_1 \\ \lambda_2^{(M-K+1)} = \lambda_2^{(M-K)} = \cdots = \lambda_2^{(M-K-r+2)} &= W_2 \end{aligned}\right\} \tag{2.7}$$

where r is the order of the eigenvalue $\lambda_1^{(K)}$ for $\mathcal{D}_1$ and of the eigenvalue $\lambda_2^{(M-K+1)}$ for $\mathcal{D}_2$. A conclusion cannot be drawn in general. Indeed, we have $m_1 = K - 1$, $m_2 = M - K - r + 1$, and the total number of C.R. to be used at P is $M - m_1 + M - m_2 = M + r$. The velocity W_1 of Σ being obtained from (2.7), the problem of the matching of $\mathcal{D}_1$ and $\mathcal{D}_2$ is well-posed only if r jump relations (among the M jump relations) are degenerate, i.e. are automatically satisfied. This is the case for a slip surface when the full system of Euler's equations is solved.

3 - PRACTICAL IMPLEMENTATION OF THE COMPATIBILITY RELATIONS FOR THE DISCRETIZED PROBLEM -

The numerical method used (see part II) is based on the equations in conservative form :

$$\frac{\partial U}{\partial t} + \frac{\partial F_j(U)}{\partial x_j} = 0 \tag{3.1}$$

where U is the vector of the conservative variables, and the F_j (j = 1, 2, 3) are the corresponding fluxes.

Knowing U(f), the matrices A_j of formulation (1.1) are given by :

$$A_j = A_0^{-1} \frac{\partial F_j}{\partial U} A_0 \tag{3.2}$$

where

$$A_0 = \partial U / \partial f \tag{3.3}$$

Then the C.R. (1.5) assume the form :

$$\alpha^{(k)} \cdot A_0^{-1} \cdot \left(\frac{\partial U}{\partial t} + \frac{\partial F_j}{\partial x_j} \right) = 0 \tag{3.4}$$

At inner mesh points, the discretized equations can be written :

$$U^{n+1} - U^n = - \Delta t \left(\delta F_j / \delta x_j \right)^{n+1/2} \tag{3.5}$$

where $(\delta F_j / \delta x_j)^{n+1/2}$ stands for a discrete approximation of $(\partial F_j / \partial x_j)$ at time $(n + \frac{1}{2}) \Delta t$ at the mesh point considered. At a boundary point P of a subdomain $\mathcal{D}_1$, some C.R. are used and the discrete forms of these C.R. can be obtained most conveniently as follows. First, all the equations of system (3.1) are discretized at P, in the form (3.5) except for the fact that the scheme must be suitably modified in order to involve only mesh points in $\mathcal{D}_1$ and on the boundary Γ_1. Let us note U* the value thus obtained at P ; it verifies :

$$U^* - U^n = - \Delta t \left(\bar{\delta} F_j / \delta x_j \right)^{n+1/2} \qquad (3.6)$$

where the bar on $\bar{\delta}$ is to recall that the scheme is modified compared to the current scheme at inner points.

On the other hand, a formal discretization of the C.R. (3.4) at P yields :

$$\left[\alpha^{(k)} \cdot A_0^{-1} \right]^{n+\frac{1}{2}} \cdot \left[\frac{U^{n+1} - U^n}{\Delta t} + \left(\frac{\bar{\delta} F_j}{\delta x_j} \right)^{n+\frac{1}{2}} \right] = 0 \qquad (3.7)$$

By eliminating the discretized flux terms between (3.6) and (3.7), we obtain the simple form of the discretized C.R. :

$$\left[\alpha^{(k)} \cdot A_0^{-1} \right]^{n+\frac{1}{2}} \cdot \left[U^{n+1} - U^* \right] = 0 \qquad (3.8)$$

The value of U^{n+1} at P is obtained as the solution of a set of discrete equations made of the discretized C.R. used at P, of the form (3.8), and of the discrete boundary conditions or matching conditions.

It turns out that the discretized C.R. assume a much simpler form if expressed in terms of judiciously chosen non-conservative variables f (ρ , $\vec{V}$,p for the full Euler system) instead of the conservative variables U. From (3.3), we see that (3.8) can be written, to second-order :

$$\alpha^{(k)\, n+\frac{1}{2}} \cdot \left[f^{n+1} - f(U^*) \right] = 0 \qquad (3.9)$$

In practice, we have evaluated $\alpha^{(k)}$ at time $n \Delta t$ instead of time $(n + \frac{1}{2}) \Delta t$.

Part II

Multi-Domain Euler or Navier-Stokes

Calculations of Transonic Flows

1 - NUMERICAL SCHEME -

We use an adaptation of the explicit MacCormack scheme [10] with direct discretization in the physical plane in arbitrary meshes.

Two types of artificial viscosity are implemented. The non-linear artificial viscosity term of Lerat-Sides [11] is used for shock capturing (but restricted to the mesh line direction approximately parallel to the flow). A linear fourth-order artificial viscosity term is used to damp short wave-length instabilities in particular in the viscous layers. This latter viscosity is not sensitive to the high transverse gradients encountered in the viscous layers.

In the case when the shock-fitting technique is implemented, the shock is a moving mesh line, of the family i = cst, so that all the mesh lines i = Cst move with the shock (with decreasing amplitude as the distance from the shock increases). The approach followed here to take the mesh motion into account is to consider that the discrete equations apply in the mesh frozen at time $t_n = n\,\Delta t$, and to advance the solution from t_n to $t_{n+1} = t_n + \Delta t$ in this frozen mesh. The new mesh at time t_{n+1} is then calculated, and the numerical solution at time t_{n+1} is transfered from the old mesh to the new mesh using a simple first order Taylor's expansion. This technique is only first-order accurate for the transient stage, but second-order accuracy is recovered at the steady state.

Details about the numerical method can be found in Refs. [1] , [12] and [13] .

2 - ZONAL MESH REFINEMENT IN A VISCOUS LAYER -

Very high mesh refinements are required in viscous layers at large Reynolds numbers. The technique commonly used is to make a coordinate transformation based on an analytical stretching function (e.g. exponential function). If this analytical refinement is too rapid, or equivalently if the number of mesh points is not large enough, then the local mesh size refinement ratio may be much larger than unity, and this can lead to truncation errors much larger than the theoretical truncation error determined with the assumption of a uniform mesh.

Here we use a technique introduced by Viviand and Ghazzi [14] and which combines a mild analytical stetching with a dichotomy technique. First we define a basic mesh based (in two dimensions) on a chosen curvilinear coordinate system (ξ , η) such that $\eta = 0$ represents the wall, and the viscous layer is contained within a region defined by $0 \leq \eta \leq \eta_e$ (Cst.).

The basic mesh includes the effect of a stretching function g (Y), and the mesh lines following the wall direction are :

$$Y = Y_j = (j-1)\,\Delta Y \quad , \quad j = 1, 2, \ldots J+1 \tag{2.1}$$

when η is related to Y by the stretching function :

$$\eta = \eta_e\, g(Y) \quad , \quad g(0) = 0 \quad , \quad g(1) = 1 \tag{2.2}$$

where g (Y) must be an increasing function.

A classical form for the stretching function is the exponential :

$$g(Y) = \frac{e^{\beta Y} - 1}{e^{\beta} - 1} \quad , \quad \beta > 0 \tag{2.3}$$

The local mesh refinement ratio, for the basic mesh, is then a constant r :

$$(\eta_{j+1} - \eta_j)/(\eta_j - \eta_{j-1}) = r = e^{\beta \Delta Y} \qquad (2.4)$$

The global mesh refinement ratio is then :

$$(\eta_{J+1} - \eta_J)/(\eta_2 - \eta_1) = R_B = r^{J-1} = e^{\beta(1-\Delta Y)} \qquad (2.5)$$

The dichotomy technique applies on this basic mesh which is uniform in the Y-variable. Starting from this basic mesh, the number of mesh lines Y = Cst is doubled (corresponding to halving the mesh size in Y) repeatedly in embedded regions of the type $0 < Y < Yn$ with $Yn+1 < Yn$; n is thus equal to the total number of dichotomies operated upon the basic Y-mesh in the region $Yn+1 < Y < Yn$. The resulting mesh has a zonal structure in Y, such that each zone has a uniform mesh size in Y, and such that adjacent zones overlap as shown on Fig. 1. These zones are referred to by a superscript q (q = 1 to Q) increasing from the wall Y = 0 to the outer boundary Y = 1. The mesh size in Y for zone q is thus $\Delta Y^{(q)} = 2^{q-Q}\,\Delta Y$. Zone Q in the upper part of the domain is simply what is left of the basic mesh. An example of such a zonal mesh, with Q = 6, is shown on Fig. 2.

With the dichotomy technique, the global mesh refinement ratio is now found to be :

$$R_G = \Delta\eta^{(Q)}_{L(Q)} / \Delta\eta^{(1)}_2 = e^{\beta}\left(1 - \frac{1}{r}\right)/\left(r^{2^{1-Q}} - 1\right) \qquad (2.6)$$

where $\Delta\eta^{(q)}_\ell = \eta^{(q)}_\ell - \eta^{(q)}_{\ell-1}$, the index ℓ being a local numbering of the mesh lines Y = cst in a given zone, with $1 \leq \ell \leq L^{(q)}$ for zone q. (so that $\eta^{(q)}_1 = 0$, $\eta^{(Q)}_{L(Q)} = \eta_e$).

For a given value of β , i.e. a given stretching function g (Y), and for a fixed global mesh refinement ratio (i.e. $R_B = R_G$), the dichotomy technique allows a reduction in the total number of mesh lines Y = Cst. Moreover the local mesh refinement ratio, which is a constant in each zone, say $r^{(q)}$ for zone q, decreases and becomes closer to 1 as q decreases (i.e. as the wall is approched); we have :

$$r^{(q)} = \sqrt{r^{(q+1)}} = r^{2^{q-Q}} \qquad (2.7)$$

This is a very favourable feature for accuracy since the mesh is more uniform in η in zones close to the wall where the highest transverse gradients are encountered.

Of course, the discretization of the equations must remain interior to each zone : with the Navier-Stokes equations, the MacCormack scheme can be applied in zone q only on the mesh lines $\ell = 3$ to $\ell = L^{(q)} - 2$. The problem then arises of matching the solutions in adjacent zones. This problem is solved by making the zones overlap as shown on Fig. 1. The values $U^{(q)}_\ell$ of the unknown U on the lines $\ell = 1,2,\ L^{(q)} - 1,\ L^{(q)}$ of zone q are then determined from the calculated values of U in the adjacent zones (q - 1) or (q + 1) by means of the relations :

$$U^{(q)}_1 = U^{(q-1)}_{L^{(q-1)}-4} \quad , \quad U^{(q)}_2 = U^{(q-1)}_{L^{(q-1)}-2} \qquad (2.8)$$

$$\left.\begin{aligned} U^{(q)}_{L^{(q)}} &= U^{(q+1)}_{3} \\ U^{(q)}_{L^{(q)}-1} &= \frac{1}{16}\left\{-U_1 + 9\left(U_2 + U_3\right) - U_4\right\}^{(q+1)} \end{aligned}\right\} \quad (2.9)$$

3 - ZONAL TIME-MARCHING PROCEDURE -

Due to the very small mesh size at the wall, advancing the solution in time with the same time-step in all the zones would be extremely costly with an explicit scheme, since that time-step would be the one fixed by stability conditions in the wall region.

Advantage can be taken of the zonal structure of the mesh to use different time-steps in different zones. Practically, we found that we could use a time-step proportional to the mesh size in Y, so that the time-step $\Delta t^{(q)}$ used in zone q is given by :

$$\Delta t^{(q)} = 2^{q-Q}\ \Delta t \quad (2.10)$$

where Δt is the time-step used in the outer zone Q.

A systematic sweeping procedure has been set up to advance the solutions in time in a regular way in the different zones. The diagram of Fig. 3 explains this procedure for one cycle, i.e. the set of time iterations carried out in all the zones (here 4 zones) to advance the solution in time of Δt in all the zones. Following the circles gives the order in which the zones are swept and the time-level reached in each zone. The small arrows near each circle indicate the matching with the adjacent zones above ($\longrightarrow$) or below ($\longleftarrow$) according to the relations (2.8), (2.9), the latest calculated walues in a zone being always transferred to the zone below, but conditionally transferred to the zone above.

4 - EXAMPLES -

Applications of this multi-domain approach to inviscid flow calculations, based on the Euler equations, and to viscous flow calculations, based on the Navier-Stokes equations, will be presented. In the latter case, the matching boundaries between sub-domains must be located in regions where viscous effects are negligible.

An example of inviscid flow calculation is given on Figs. 4 and 5. It concerns the transonic flow past the NLR 7301 profile at Mach number $M_\infty = 0.721$ and incidence $\alpha = -0.194°$ (design conditions). The computation domain is divided into 6 sub-domains shown on Fig. 4 with the corresponding meshes. A first partitioning is to separate the upper and the lower half-planes by means of two cut-lines which are the upstream x-axis on the one hand, and the streamline (which can be a slip-line) issued from the trailing-edge, which is thus fitted. Figure 5 shows the iso-Mach lines. A very weak and short shock forms on the upper surface, hence a very small Mach number jump across the streamline issued from the trailing-edge. Despite the large variations in mesh size from one sub-domain to another, the iso-Mach lines pattern remains smooth across the inner boundaries.

The second example concerns the numerical simulation of the interaction between a shock and a turbulent boundary layer in a transonic plane channel, based on the time-averaged Navier-Stokes equations and a mixing-lenght type turbulence model. Figure 6.a shows the computation domain (the upper boundary is a symmetry axis) which is divided into 3 sub-domains. In the two upper sub-domains $\mathcal{D}_f^{(1)}$ and $\mathcal{D}_f^{(2)}$, the viscous effects are quite negligible and the Euler equations are used. The inner boundary Σ_2 between $\mathcal{D}_f^{(1)}$ and $\mathcal{D}_f^{(2)}$ is made of the shock which is thus fitted in this upper part of the channel. The Navier-Stokes equations are used in the lower sub-domain $\mathcal{D}_v$ where the shock is captured. In $\mathcal{D}_v$ the mesh is refined near the wall by using the dichotomy technique as described in § 2. The actual zonal mesh structure, in the physical plane, is shown on Fig. 2. The computed flow field is shown on Figs. 6.b to 6.d which give maps of iso-Mach lines, isobars and iso-density lines ; the latter can be compared with an experimental flow visualization by interferometry shown on Fig. 6.e.

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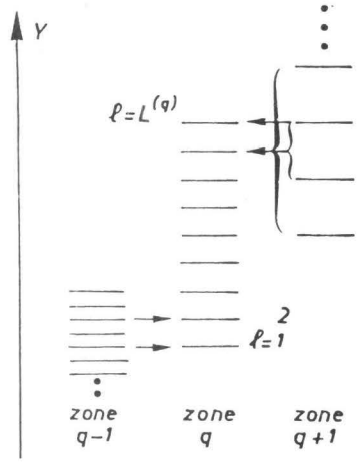


Fig.1 - Dichotomy technique and matching of zones

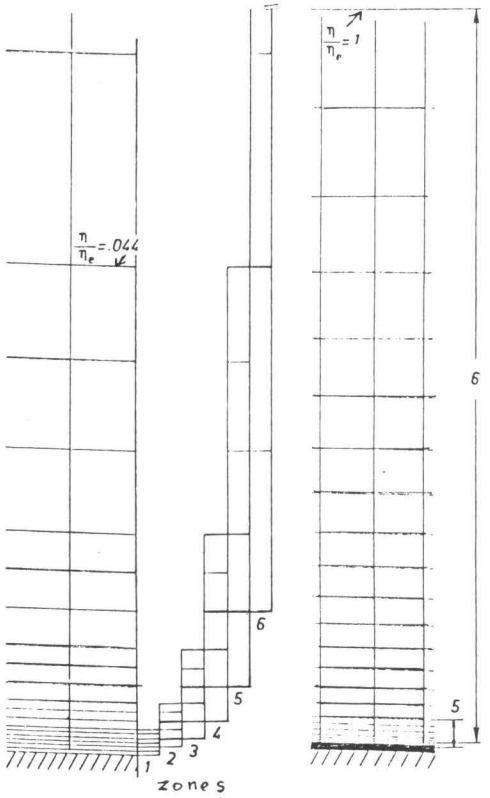


Fig.2 - Mesh lines Y = Cst. in the physical plane and zonal structure (Q = 6)

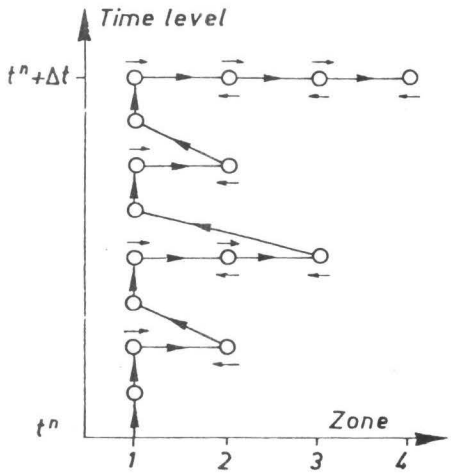


Fig.3 - Zonal time-marching procedure and matching. Iterations for 1 cycle with Q = 4

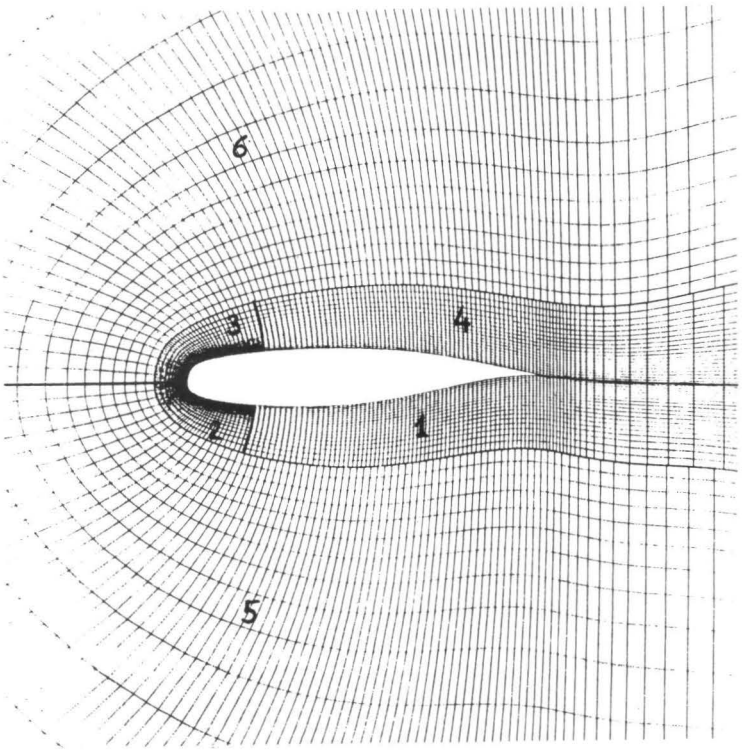


Fig.4 - NLR 7301 profile. Decomposition into 6 sub-domains and corresponding meshes

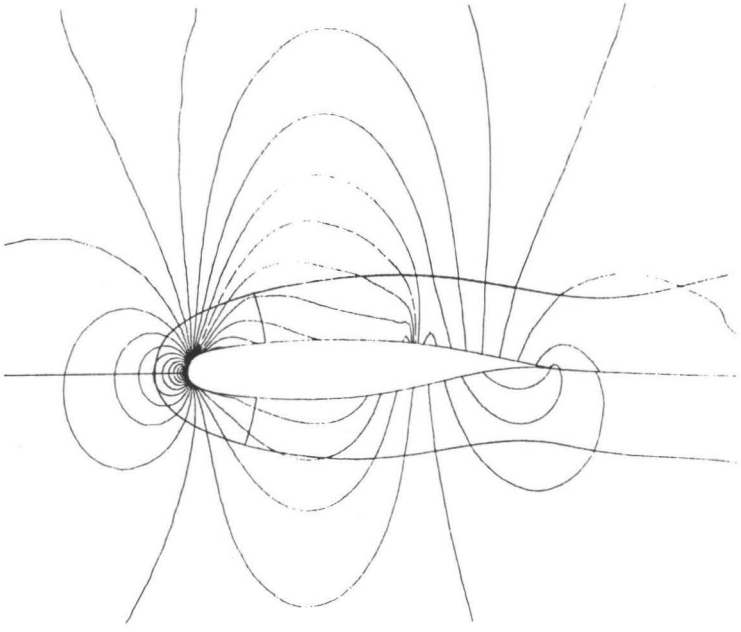
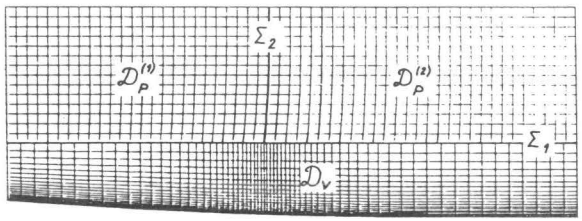
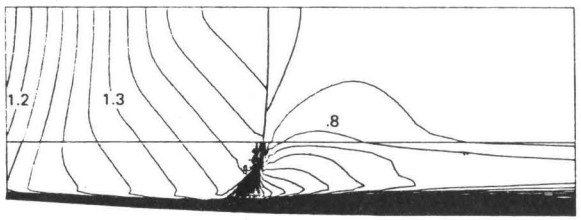


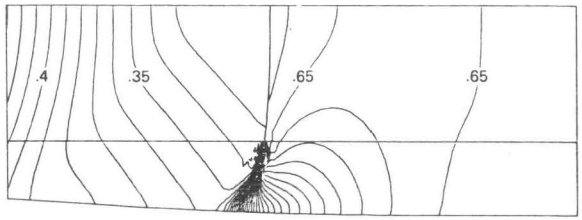
Fig.5 - NLR 7301 profile - $M_\infty = 0.721$, $\alpha = -0.194°$
Iso-Mach lines ($\Delta M = 0.02$)



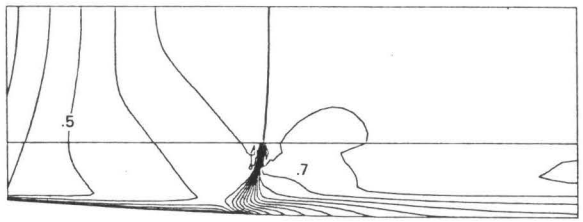
a) Computation domain and meshes in the 3 sub-domains



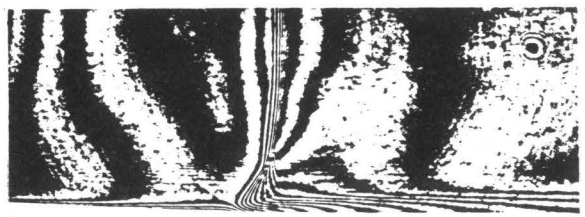
b) Iso-Mach lines ($\Delta M = 0.02$)



c) Isobars ($\Delta p = 0.01\ p_{i_0}$)



d) Iso-density lines ($\Delta \rho = 0.02\ \rho_{i_0}$)



e) Experiment (interferometry)

Fig.6 - Shock-boundary layer interaction in a plane transonic channel

The Numerical Solution of Large Sparse Nonsymmetric Linear Systems

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Lecture No. 1. Introduction to Iterative Algorithms for Solving Nonsymmetric Linear Systems

Lecture No. 2. Iterative Algorithms and Software for Solving Large Sparse Nonsymmetric Linear Systems

We consider iterative algorithms for solving the linear system

$$Au = b \tag{1}$$

where A is a given square matrix of order N and b is a given column vector. It is assumed that, as in the case where one is solving an elliptic boundary value problem by a discretization method, the matrix A is very large and very sparse. We will be primarily concerned with cases where the matrix A is nonsymmetric, or is symmetric but not symmetric and positive definite (SPD).

There are a number of effective iterative algorithms for solving (1) for the case where A is SPD. Such algorithms normally involve the use of a basic iterative method combined with an acceleration procedure. The basic iterative method has the form

$$u^{(n+1)} = Gu^{(n)} + k \tag{2}$$

where $G = I - Q^{-1}A$, $k = Q^{-1}b$ for some nonsingular matrix Q, sometimes known as the "splitting" matrix. Alternatively, one can derive (3) from a given

Q by first constructing the preconditioned system

$$Q^{-1}Au = Q^{-1}b \tag{3}$$

by multiplying both sides of (1) by Q^{-1}. The method (2) can be obtained from (3) by using a (second) splitting matrix $Q' = I$. All of the standard basic iterative methods (Richardson, Jacobi, Gauss-Seidel, SOR, SSOR, incomplete Cholesky, etc.) can be obtained in this way for suitable choice of the splitting matrix Q.

If the matrix A of the system (1) is SPD then most of the standard basic iterative methods are symmetrizable, i.e., $I - G$ is similar to an SPD matrix or, equivalently, $Z(I - G)$ is SPD for some SPD matrix Z. For most standard basic iterative methods Q is SPD whenever A is SPD and one can let $Z = Q$ or $Z = A$. The iteration matrix G of a symmetrizable iterative method has two important properties: the eigenvalues of G are real and less than one; the Jordan canonical form of G is a diagonal matrix.

The speed of convergence of a symmetrizable basic iterative method can be increased by an order of magnitude by the use of an acceleration procedure such as Chebyshev acceleration or one of several alternative forms of conjugate gradient acceleration. Moreover adaptive procedures can be used to determine any parameters which are needed for the basic iterative method and for the acceleration procedure; see, e.g., Hageman and Young [1981]. In addition, realistic procedures have been developed for terminating the iterative procedure. A software package, known as ITPACK, has been developed for solving systems of the form (1), where A is SPD, by a variety of iterative algorithms; see Kincaid et al. [1982].

In the case where the matrix A of (1) is not SPD (we refer to this case as the nonsymmetric case), the standard basic iterative methods are not symmetrizable. The eigenvalues of the iterative matrix G may be

complex and, moreover, the Jordan canonical form of G may not be diagonal; hence there may no longer exist a basis of eigenvectors of G. This complicates the use of acceleration procedures and the determination of iteration parameters.

The primary purpose of these talks is to describe some of the methods which have been developed for treating the nonsymmetric case. These include: the (unaccelerated) SOR method; the GCW method (where $Q = \frac{1}{2}(A + A^T)$) combined with acceleration; the use of various normal equations together with acceleration; and the use of Chebyshev, Krylov subspace and Lanczos acceleration procedures applied to basic iterative methods.

One procedure for handling nonsymmetric systems is the SOR method. If A is a consistently ordered matrix whose eigenvalues have positive real parts, then the SOR method converges for some values of ω, and if the eigenvalues of the matrix B corresponding to the Jacobi method are available then one can determine an optimum value of the relaxation factor ω; see, e.g., Rigal [1979], Young and Huang [1983] and Huang [1983].

Ehrlich [1984] considered the use of "ad hoc" SOR. Ad hoc SOR can be used for elliptic difference equations and involves the use of a different ω for each mesh point. At each mesh point the value of ω is computed based on the values of the coefficients of the differential equation at that point and on the size of the region. Good results have been obtained using this method for many problems.

Concus and Golub [1976] and Widlund [1978] considered the use of a basic iterative method, which we will call the GCW method, which corresponds to the splitting matrix $Q = \frac{1}{2}(A + A^T)$. This scheme is intended for the case where A is PR (i.e., where $A + A^T$ is SPD) and

where one can conveniently solve intermediate linear systems involving Q, for example, by fast direct methods. It can be shown that, even though the GCW method is not symmetrizable, nevertheless, many of the acceleration procedures described below become as simple when applied to the GCW method, as they are in the symmetrizable case. The GCW method is particularly effective in the case where the eigenvalues of the iteration matrix G have small imaginary parts.

Given a linear system (1) with a matrix A which is nonsingular but not necessarily SPD one can construct an equivalent linear system with an SPD matrix by multiplying both sides of (1) by A^T obtaining the normal equations $A^TAu = A^Tb$. Evidently the matrix of the new system is SPD. Hence one can apply an acceleration procedure. However, in general the condition number of A^TA, which governs the convergence rate, is much larger than that of A. In many cases an acceleration method applied to a basic iterative method for the normal equations is no faster than an unaccelerated basic iterative method applied to the original system (1). Because of this it is usually wise to avoid the use of the normal equations wherever possible.

Dongarra et al. [1981] and Elman [1982] considered the use of generalized normal equations based on the preconditioned system (2). This leads to the system $(I - G)^T(I - G)u = (I - G)^Tk$. Other, slightly more general normal equations are considered by Young, Jea and Kincaid [1984] and by Elman [1982]. In some cases the condition of the matrix for the matrix corresponding to the generalized normal equations may not be too much greater than for the preconditioned system. This is true in some cases, as shown in Young, Jea and Kincaid [1984] for the generalized normal

equations corresponding to the SOR method. These generalized normal equations correspond to the SSOR method. It should be noted that the SSOR method with conjugate gradient acceleration converges much faster than the SOR method in some cases. In such cases the condition number for the generalized normal equations is only slightly larger than for the original system.

Krylov subspace methods are an important class of methods for accelerating the convergence of nonsymmetrizable basic iterative methods. Basically, starting with an arbitrary initial vector $u^{(0)}$ one considers the Krylov space $K_n(\delta^{(0)}) = Sp\{\delta^{(0)}, Q^{-1}A\delta^{(0)}, \ldots, (Q^{-1}A)^{n-1}\delta^{(0)}\}$ spanned by the vectors $\delta^{(0)}, Q^{-1}A\delta^{(0)}, \ldots$. Here $\delta^{(0)} = Q^{-1}(b - Au^{(0)})$. At each step the vector $u^{(n+1)}$ is chosen so that $u^{(n)} - u^{(0)} \in K_n(\delta^{(0)})$ and so that some other condition is satisfied. Examples of such conditions include a variational condition that $u^{(n)} - \bar{u}$ is minimized in some norm and a Galerkin condition that $u^{(n)} - u^{(0)}$ is orthogonal, in some sense, to each vector v of $K_n(\delta^{(0)})$.

Young and Jea [1980] considered a family of Krylov subspace methods which we shall refer to as IGCG methods. The application of these methods involves the use of an auxiliary matrix Z. For simplicity let us assume that Z(I - G) is PR. If we apply a modified Gram-Schmidt orthogonalization procedure to the Krylov vectors $\delta^{(0)}$, $(I - G)\delta^{(0)}$, ..., where $\delta^{(0)} = Gu^{(0)} + k - u^{(0)}$, to obtain the direction vectors $q^{(0)}$, $q^{(1)}$, ..., and then apply the Galerkin condition we obtain the following method, called ORTHODIR,

$$u^{(n+1)} = u^{(n)} + \hat{\lambda}_n q^{(n)}; \quad q^{(n)} = (I - G)q^{(n-1)} + \beta_{n,n-1}q^{(n-1)} + \ldots + \beta_{n,0}q^{(0)}$$

where $\hat{\lambda}_n$ and the $\beta_{n,i}$ can be computed explicitly. This method can be shown to converge, in theory, if Z(I - G) is PR. By direct algebraic

transformations one can obtain two equivalent forms, namely ORTHOMIN which has the form

$$u^{(n+1)} = u^{(n)} + \lambda_n p^{(n)}; \quad p^{(n)} = \delta^{(n)} + \alpha_{n,n-1} p^{(n-1)} + \ldots + \alpha_{n,0} p^{(0)}$$

where $\delta^{(n)} = Gu^{(n)} + k - u^{(n)}$, and ORTHORES which has the form

$$u^{(n+1)} = \lambda_n \delta^{(n)} + f_{n+1,n} u^{(n)} + \ldots + f_{n+1,0} u^{(0)}$$

ORTHOMIN and ORTHORES converge if both Z and Z(I - G) are PR. ORTHOMIN most closely resembles the standard form of the conjugate gradient matrix, see Hestenes and Stiefel [1952], while ORTHORES resembles the form used by Engeli et al. [1959].

In actual practice it is usually not feasible to use the IGCG methods in their complete form because of the very large storage and machine time which would be required. One procedure is to truncate, i.e., to disregard all terms except those relating to the n, n-1, ..., n-s iterations. This leads to ORTHODIR(s), ORTHOMIN(s) and ORTHORES(s). Unfortunately many of the convergence properties of the methods may be lost if truncation is used. Another procedure is to use the complete formulas but to restart the calculation periodically.

Saad and Schultz [1983] presented an abstract framework of methods which included most Krylov subspace methods. In addition to the IGCG methods, the procedures considered included the generalized conjugate residual method (see Elman [1982]), a least squares method of Axelsson [1980a], a generalized minimum residual method (GMRES) of Saad and Schultz [1983a], the full orthogonalization method of Saad [1981] and a method of Axelsson [1980] based on a Galerkin method. Truncated and restarted versions of the methods were also considered. Many of these schemes are mathematically, though not necessarily computationally, equivalent to IGCG methods.

Saad [1980] also considered a Krylov subspace method based on the method of Arnoldi [1951].

In some cases the formulas for the IGCG methods simplify. If ORTHODIR, ORTHOMIN, and ORTHORES resude to ORTHODIR(s+1), ORTHOMIN(s), and ORTHORES(s) we have a simplification of degree s. In the symmetrizable case if the auxiliary matrix Z is chosen so that Z and Z(I - G) are SPD then we have a simplification of degree one. It can also be shown, see Jea [1982] and Jea and Young [1983] that if I - G is similar to a symmetric matrix then simplification of degree one occurs for suitable Z. Moreover, it can also be shown that ORTHODIR(2) converges, at least in the absence of roundoff. Finally, it follows from results of Faber and Manteuffel [1984] that if I - G is similar to a normal matrix, then for some integer s we obtain a simplification of degree s for suitable Z. Also, a partial converse to the last result follows from the work of Faber and Manteuffel. Thus, it can be shown that, except for certain special cases, a simplification of degree s occurs for some auxiliary matrix Z such that Z(I - G) is SPD only if I - G is similar to a normal matrix. This result answers a question raised by Golub [1981] and rules out the possibility that in the general case one can choose an auxiliary matrix Z such that Z(I - G) is SPD and such that there is simplification.

In spite of the above result, it is in theory possible to obtain a simplification of degree one. Jea [1982] and Jea and Young]1983] showed that there always exists a symmetric matrix H such that $H(I - G) = (I - G)^T H$. (If H were SPD then I - G would be similar to a symmetric matrix and we would be assured of the convergence of ORTHODIR(2) from the result stated previously.) It can be shown that a simplification of degree one occurs using Z = H. Unfortunately it is, in general, not feasible to find H. Also, even if H were known, there is no guarantee that the method would not break down.

On the other hand, as shown by Jea and Young [1983], by applying this procedure to an expanded linear system one can derive a version of the Lanczos method corresponding to each of the three IGCG methods.

We refer to the three versions of the Lanczos method, derived as described above, as the Lanczos/ORTHODIR, Lanczos/ORTHOMIN and Lanczos/ORTHORES methods. The Lanczos/ORTHOMIN method has the form $u^{(n+1)} = u^{(n)} + \lambda_n p^{(n)}$, where $p^{(n)} = \delta^{(n)} + \alpha_n p^{(n-1)}$, $\tilde{p}^{(n)} = \tilde{\delta}^{(n)} + \alpha_n \tilde{p}^{(n-1)}$, $\delta^{(n+1)} = \delta^{(n)} - \lambda_n Q^{-1}Ap^{(n)}$, $\tilde{\delta}^{(n+1)} = \tilde{\delta}^{(n)} - \lambda_n (Q^{-1}A)^T \tilde{p}^{(n)}$. Here $u^{(0)}$ and $\tilde{\delta}^{(0)}$ are arbitrary and $\delta^{(0)} = Gu^{(0)} + k - u^{(0)}$. The Lanczos/ORTHOMIN method is equivalent to the biconjugate gradient method presented by Fletcher [1976]. Each form of the Lanczos method has the advantage of requiring information only from the nth and (n-1)st iteration. Unfortunately, however, the method may break down.

Chebyshev acceleration can be applied to a basic iteration provided that the eigenvalues of the iteration matrix G have real parts less than unity. Manteuffel [1977] developed a procedure for determining the optimum parameters needed for Chebyshev acceleration in terms of the (complex) eigenvalues of G. This involves the determination of numbers a, b and d such that all eigenvalues of G lie in the ellipse $((x-d)/a)^2 + (y/b)^2 = 1$ and such that the quantity $S = (a+b)[1 - d + \sqrt{(1-d)^2 + 1^2}]^{-1}$ is minimized An alternative procedure is given by Huang [1983]. Manteuffel [1978] gave a procedure for estimating key eigenvalues of G based on the results of previous iterations. Elman, Saad, and Saylor [1984] developed a "hybrid" scheme involving Chebyshev acceleration and the estimation of key eigenvalues using GMRES; see Saad and Schultz [1983a]. At Texas we are working on another hybrid scheme based on the use of the Lanczos method to find the key eigenvalues of G.

Numerical experiments based on Manteuffel's algorithm with various preconditionings based on approximate factorization methods are described by Van der Vorst [1981].

In some cases the eigenvalue spectrum of the iteration matrix G is not well approximated by an ellipse. For such cases polynomials other than Chebyshev polynomials are used; see Smolarski [1981], Smolarski and Saylor [1982], Saylor [1981], and Opfer and Schober [1984].

There are relatively few general theoretical results concerning the methods which have been described above for solving nonsymmetric systems. It therefore seems appropriate that, while continuing to search for theoretical results, one should also try the experimental approach. To this end two software packages have been developed: the (new) Yale sparse matrix package (see Eisenstat et al. [1984]), and the ITPACK 3 package which is being developed at Texas.

ITPACK 3, which is being developed by T.S. Mai, is a research-oriented software package designed to be used as a research tool in the study of methods for solving nonsymmetric linear systems. A preliminary version, called ITPACK 3A, will soon be available for informal distribution. The program can be instructed to apply any one of several acceleration procedures to any one of several basic iterative methods using any auxiliary matrix Z. Various adaptive procedures can be used to determine any necessary iteration parameters.

The ITPACK 3A package has been used to carry out some numerical experiments, see Abbassian [1984]. It has also been used in graduate courses in numerical analysis.

The full ITPACK 3 package, when complete will allow the user to employ more sophisticated procedures. For example, a hybrid scheme involving Chebyshev acceleration can be used and the Lanczos method where the Chebyshev parameters would be periodically updated using the Lanczos method.

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