CONFERENTIE VAN NUMERIEK WISKUNDIGEN

5 oktober - 7 oktober 1987

CONFERENTIEOORD WOUDSCHOTEN
ZEIST

Werkgemeenschap Numerieke Wiskunde

CONFERENTIE VAN NUMERIEK WISKUNDIGEN

Werkgemeenschap Numerieke Wiskunde

TWAALFDE 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. *Het numeriek oplossen van bifurcatieproblemen, en homotopiemethoden.*

2. *Hyperbolische differentiaalvergelijkingen en zwak reflecterende randen.*

Organisatie

De organisatie is in handen van de voorbereidingscommissie bestaande uit de heren Traas (UT) (voorzitter), van der Sluis (RUU), van der Vorst (TUD) en Hundsdorfer (CWI) (secretaris), en van het Centrum voor Wiskunde en Informatica.

Uitgenodigde Sprekers

Thema 1. H.D. Mittelmann, Arizona State University, Tempe, USA.
H. Schwetlick, Martin-Luther-Universität, Halle, DDR.
A. Spence, University of Bath, U.K.

Thema 2. B. Gustafsson, Uppsala University, Sweden.
A. Lerat, E.N.S.A.M., Paris, France.
P.L. Roe, Cranfield Institute of Technology, U.K.

Een korte voordracht zal worden gegeven door F.P.H. van Beckum, J.I. van den Berg, M. van Veldhuizen en A.J.N. Vreenegoor.

Programma

Maandag 5 oktober

10.00-11.15	aankomst, koffie	15.15-15.45	thee
11.15-12.15	opening, Gustafsson	15.45-16.45	Lerat
12.30	lunch	16.50-17.20	van Veldhuizen
14.15-15.15	Mittelmann	18.00	diner

Dinsdag 6 oktober

-8.00	ontbijt	14.15-15.15	Gustafsson
-9.00-10.00	Schwetlick	15.15-15.45	thee
10.00-10.30	koffie	15.45-16.45	Mittelmann
10.30-11.30	Roe	16.50-17.20	Vreenegoor
11.35-12.35	Spence	17.20-17.50	Vergadering Werkgemeenschap Numerieke Wiskunde
12.45	lunch		
		18.00	diner

Woensdag 7 oktober

-8.00	ontbijt	12.05-12.35	van Beckum
-9.00-10.00	Lerat	12.45	lunch
10.00-10.30	koffie	13.45-14.45	Roe
10.30-11.30	Schwetlick	14.50-15.50	Spence
11.35-12.05	van den Berg	15.50	sluiting, thee, vertrek

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

Titels en Samenvattingen Voordrachten

Maandag 5 oktober

11.15	opening	
	B. Gustafsson	*Nonreflecting boundary conditions for the wave equation. Well-posedness and stability*
14.15	H.D, Mittelmann	*Continuation methods for parameter-dependent boundary value problems*
15.45	A. Lerat	*A unified presentation of difference schemes for hyperbolic systems of conservation laws*
16.50	M. van Veldhuizen	*On numerical methods for invariant curves*

Dinsdag 6 oktober

9.00	H. Schwetlick	*Basic techniques in path following algorithms and applications to homotopy methods*
10.30	P.L. Roe	*Weakly reflecting boundary conditions for external aerodynamic problems*
11.35	A. Spence	*The numerical computation of bifurcation points arising in the finite Taylor problem*
14.15	B. Gustafsson	*Far field boundary conditions for first order systems. Applications to the Euler equations*
15.45	H.D. Mittelmann	*Continuation methods for parameter-dependent boundary value problems*
16.50	A.J.N. Vreenegoor	*A numerical study of nonlinear wave-interactions in bubbly two-phase flow*

Woensdag 7 oktober

9.00	A. Lerat	*An implicit centered scheme without artificial viscosity for the calculation of steady compressible flows with shocks*
10.30	H. Schwetlick	*Numerical methods for computing turning points of nonlinear equations*
11.35	J.I. van den Berg	*Well-posedness of combining characteristic boundary conditions and conservation equations at boundaries of cell-centered 3D Euler-flow calculations*

12.05	F.P.H. van Beckum	*Discretizations conserving energy and other constants of the motion*
13.45	P.L. Roe	*Weakly reflecting boundary conditions for external aerodynamic problems*
14.50	A. Spence	*The use of singularity theory in the numerical analysis of bifurcation problems*

Discretizations conserving energy and other constants of the motion

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Various evolution equations from mathematical physics conserve one or more integrals (constants of the motion; e.g. the energy) and have solutions in the form of steadily propagating waves (e.g. solitairy waves).
In spatial discretizations these properties are generally lost. However, observing that the properties are a consequence of a certain variational structure (Poisson structure) of the evolution equation, we derive discretizations in such a way that they inherit this structure. Consequently the constants of the motion and the existence of steadily propagating waves are conserved.
Two examples concerning surface waves will be shown.

Well-posedness of combining characteristic boundary conditions and conservation equations at boundaries of cell-centered 3D Euler-flow calculations

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In the calculation of three-dimensional Euler flow with a cell-centred scheme, the formulation of the flow condition at the boundary is very important. Solving the Euler equations in the continuum case, boundary conditions can be formulated with characteristic theory. However, when solving the Euler equations numerically with a cell-centred scheme, boundary conditions are not sufficient. This leads to a underdetermined set of discrete differential equations. Hence auxiliary equations have to be defined. The choice of these equations must lead to a well-posed numerical problem. A useful set of auxiliary equations is derived by combining characteristic forms of boundary conditions with suitable discrete conservation equations at boundaries of cell-centered Euler calculations.

The basic principle is based on the eigenvector-eigenvalue decomposition of the matrix describing the time variations of the flow state at the boundary. These time variations are expressed in terms of first-variation Riemann invariants. For the time variations of first-variation Riemann invariants, suitable boundary conditions are defined, by distinguishing between incoming and outgoing information. The distinction depends on the sign (direction) of the eigenvalue of a given Riemann invariant. The boundary conditions are constructed in such a way that they only define information entering the flow domain. The auxiliary equations are constructed in such a way that they define information leaving the flow domain.

The widely used boundary conditions at a solid wall (zero normal velocity augmented with auxiliary equations defining the pressure at the wall) leads to a loss of accuracy. This causes probably the numerical boundary layer at the wall that can be observed in most calculation results. This layer seems to affect Kutta conditions (or trailing edge conditions), and leads to a too low lift on aerofoils and wings. With the introduction of the proposed boundary conditions, the order of accuracy at the wall will be increased, and so we hope to suppress the numerical boundary layer. Results of a theoretical study of the well-posedness of these proposed boundary conditions will be shown. The study is based on the distinction between elementary Fourier wave solutions that are either incoming or outgoing over the boundaries of the flow domain. The well-posedness is based on showing that solutions, exponentially growing in time but decaying in space, cannot enter the flow field through the boundary.
The proposed boundary conditions have been successfully tested in numerical experiments for one-dimensional channel flow calculations. These results will be shown together with calculation results for more-dimensional Euler flow around wing configurations.

**Nonreflecting boundary conditions for the wave equation.
Well-posedness and stability**

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I. Nonreflecting boundary conditions for the wave equation. Well-posedness and stability.

When wave propagation problems are solved numerically, it is often necessary to introduce artificial boundaries. In most cases no data are available at these boundaries, and therefore it is necessary to construct boundary conditions which in some way accounts for the behavior of the solution outside the computational domain Ω. Hence some assumption must be made which makes it possible to solve the problem exactly outside Ω, or alternatively to compute the solution approximately in a simple way. One such assumption is that the waves are propagating only in the outward direction across the boundary. This is the basis for various procedures in common use, the most general class being the absorbing boundary conditions constructed by Engquist and Majda [2], [3], see also Higdon [14]. For an illustration of the theory we use the scalar wave equation

$$\phi_{tt} = \phi_{xx} + \phi_{yy} \,. \tag{1}$$

The solutions have components of the form

$$\begin{aligned} \phi &= \hat{\phi}\, e^{i(\omega y + \xi t)} \,, \\ \hat{\phi} &= a\, e^{\pm i\sqrt{\xi^2 - \omega^2}\, x} \,, \end{aligned} \tag{2}$$

where it is assumed that $|\xi| > |\omega|$, $\xi > 0$. As the computational boundary we take the plane $x = 0$, such that the computation domain is $x \geq 0$, $-\infty < y < \infty$. The basic principle behind the absorbing boundary conditions is that outgoing waves pass through the boundary without reflection. This means that there are no solutions corresponding to the minus-sign in (2). By differentiating we obtain

$$\hat{\phi}_x = i\sqrt{\xi^2 - \omega^2}\,\hat{\phi} \,. \tag{3}$$

This is the completely absorbing boundary condition in Fourier-space. Unfortunately, when transforming back to physical space, we get a condition which is not suitable for practical computation. Rather we would like to have an expression consisting only of powers of $i\omega$ and $i\xi$, which correspond to differential operators in physical space.

Assuming that $|\omega/\xi|$ is small, which means that the wave is moving almost perpendicular to the boundary, the square-root can be approximated by ξ. This gives the *first absorbing boundary condition*,

$$\phi_x = \phi_t \,. \tag{4}$$

When including also the next term in the Taylor expansion, we arrive at the *second absorbing boundary condition*,

$$\phi_{xt} = \phi_{tt} - \tfrac{1}{2}\,\phi_{yy} \,. \tag{5}$$

Higher order conditions can be derived, but in order to avoid strong illposedness, Padé-approximations should be used for the square-root.

Higdon [13], [14] proposes the modified form

$$\left[\prod_{j=1}^{p}\left(\cos\alpha_j\frac{\partial}{\partial t}-\frac{\partial}{\partial x}\right)\right]u=0 \tag{6}$$

where $|\alpha_j|<\pi/2$. Any plane wave travelling in the outward direction at an angle of incidence $\pm\alpha_1,\ldots,\pm\alpha_p$ satisfies (6) exactly. Therefore, if some apriori knowledge of the solution is available, the angles α_j can be specified to give little reflection. For $\alpha_1=\alpha_2=0$, (6) is equivalent to (4) if $p=1$, and equivalent to (5) if $p=2$. In the latter case it is assumed that (1) holds at the boundary.

In many applications the source is outside the computational domain. In that case the boundary conditions become inhomogeneous, e.g.

$$\phi_x-\phi_t=g(y,t) \tag{7}$$

for the first condition.

It is of course necessary that the boundary conditions are such that the problem is well posed. We have already mentioned that higher order conditions may lead to strong illposedness. But there is an inherent difficulty also for the lower order ones. The theory for wellposedness [16] is based on the Fourier-Laplace transformed equations, which for (1), (7) imply

$$\begin{aligned}\hat\phi(x,\omega,s)&=e^{-x\sqrt{s^2+\omega^2}}\,\hat\phi(0,\omega,s)\,,\\ (s+\sqrt{s^2+\omega^2}\,)\,\hat\phi(0,\omega,s)&=\hat g(\omega,s)\,.\end{aligned} \tag{8}$$

The Kreiss condition necessary for wellposedness is

$$|s+\sqrt{s^2+\omega^2}|\ge\delta>0\,,\quad \mathrm{Re}\,s\ge 0\,, \tag{9}$$

which obviously is violated for $\omega=0$, $s=0$. This is a weak illposedness, and we shall show that it is possible to derive estimates which under certain conditions allow accurate solutions. However, for the second and higher order conditions the illposedness becomes stronger, and the methods are in general less robust.

For approximations using discrete versions of the absorbing boundary conditions, similar conclusions hold. It can be shown that any consistent approximation leads to a weakly unstable method. We shall derive conditions on the smoothness of the solution such that good accuracy is still obtained. However, if these conditions are violated, we shall show that the accuracy actually may deteriorate when the order of the boundary condition increases.

We end this first lecture by discussing a procedure that eliminates the weak instabilities.

Far field boundary conditions for first order systems.
Application to the Euler equations

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Consider the first order hyperbolic system

$$U_t + AU_x + BU_y = 0\,,$$

where A has ℓ positive and $(m-\ell)$ negative eigenvalues. We want to limit the computation to the right half plane, hence we need boundary conditions at $x = 0$. After a Fourier transformation in y and Laplace transformation in t we obtain

$$\hat{U}_x + Q\hat{U} = A^{-1}\,\tilde{f}\,,$$
$$Q = A^{-1}(sI + i\omega B)$$

where $\tilde{f}$ is the Fourier transform of the initial function f. It can be shown that the eigenvalues κ_j to Q split into two sets with

$$\begin{aligned} &\mathrm{Re}\,\kappa_j > 0\,, \qquad j = 1, 2, \ldots, \ell\,, \\ &\mathrm{Re}\,\kappa_j < 0\,, \qquad j = \ell+1, \ell+2, \ldots, m\,, \end{aligned}$$

for $\mathrm{Re}\,s > 0$. Thus the matrix Q can be transformed to block diagonal form

$$T^{-1}QT = \begin{bmatrix} Q^I & 0 \\ 0 & Q^{II} \end{bmatrix}$$

where Q^I is an $(\ell \times \ell)$-matrix. It can be shown that the requirement of bounded solutions for $x \to -\infty$ leads to the condition

$$[T^{-1}\,\hat{U}]^I = -\int_0^\infty e^{Q^I\sigma}[T^{-1}A^{-1}\,\tilde{f}(\sigma,\omega)]^I\,d\sigma\,.$$

This is the exact boundary condition for the problem defined in the domain $0 \le x$, $-\infty < y < \infty$, but formulated in the transformed space. For $f = 0$ it is the perfectly absorbing boundary condition by Engquist and Majda [2]. In order to get local boundary conditions in physical space, some approximation must be made.

We shall discuss certain approximations under the assumption that $|\omega/s|$ is small. For the isentropic Euler equations and subsonic flow, these conditions can be expressed in terms of divergence, vorticity and pressure gradient. The accuracy is good if the tangential second derivative of the pressure is small.

In Lecture I we demonstrated that weak instabilities necessarily occur if absorbing boundary conditions are implemented in its derivative form. Our conditions can be formulated as a generalization of these conditions. Numerical experiments show that if they are implemented in a straightforward way, the results indeed have poor accuracy. By using an integrated form we are able to prove that the problem is well posed, and the numerical experiments show a considerable increase in accuracy.

For steady state solutions, no method based on the condition that $|\omega/s|$ is small can be expected to perform well, since $\partial U/\partial t = 0$ corresponds to $s = 0$. Therefore other methods must be developed. This has been done, for example, in [5], [7], and [10], based on the form of the exact solution outside the computational domain. This leads to a coupling of all the points on the boundary, but we will show that the method still is computationally efficient.

For illustration we use the problem of computing inviscid flow around an airfoil. The flow is governed by the nonlinear Euler equations. The only approximation made (except for discretizaton of the problem) is that the differential equations are made linear with constant coefficients in the far field. The numerical experiments show that accurate solutions can be obtained with a quite small computational domain.

In a recent paper [4], Engquist and Halpern proposes a combination of absorbing and steady state conditions which gives the exact steady state solution as $t \to \infty$. One-dimensional experiments show good convergence rate to steady state as well as good accuracy in the transient phase.

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A unified presentation of difference schemes for hyperbolic systems of conservation laws

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For a hyperbolic system in one-space dimension :

$$w_t + f(w)_x = 0 \qquad (1)$$

where $w(x,t) \in \Omega \subset \mathbb{R}^m$, we consider difference schemes involving two time-levels and at most three points at the new time-level. Denoting by w_j^n the approximation value at $x_j = j\,\Delta x$ and $t_n = n\,\Delta t$ and using

$$\Delta w_j \equiv w_j^{n+1} - w_j^n,$$

these difference schemes can be expressed as :

$$\mathcal{S}(w_{j-R}^n\ ,\ w_{j-R+1}^n\ ,\ \ldots\ ,\ w_{j+R}^n\ ,\ \Delta w_{j-1}\ ,\ \Delta w_j\ ,\ \Delta w_{j+1}\ ;\ \sigma) = 0$$

where

$$\sigma = \Delta t / \Delta x$$

By assuming the schemes to be conservative and explicit or linearly implicit, they can be written as :

$$\Delta w_j = -\sigma\,(h_{j+\frac{1}{2}} - h_{j-\frac{1}{2}})$$

with the numerical flux :

$$h_{j+\frac{1}{2}} = g_{j+\frac{1}{2}} + (H_0)_{j+\frac{1}{2}}\,\Delta w_j + (H_1)_{j+\frac{1}{2}}\,\Delta w_{j+1}$$

where the m-component vector $g_{j+\frac{1}{2}}$ and the m x m matrices $(H_0)_{j+\frac{1}{2}}$ and $(H_1)_{j+\frac{1}{2}}$ depend on $w^n_{j-R+1}, w^n_{j-R+2}, \ldots, w^n_{j+R}$ and σ.

Moreover, if we suppose that :

$$g(w^n_{j-R+1}, \ldots, w^n_{j-1}, u, u, w^n_{j+2}, \ldots, w^n_{j+R} ; \sigma) \equiv f(u),$$

i.e. we use "essentially 3-point schemes", then there exists three m x m matrices :

$$M_{j+\frac{1}{2}} = M(w^n_{j-R+1}, \ldots, w^n_{j+R} ; \sigma)$$

$$P_{j+\frac{1}{2}} = P(w^n_{j-R+1}, \ldots, w^n_{j+R} ; \sigma)$$

$$Q_{j+\frac{1}{2}} = Q(w^n_{j-R+1}, \ldots, w^n_{j+R} ; \sigma)$$

such that the schemes can be put in the simple form :

$$\begin{aligned} &\Delta w_j + \frac{\sigma}{2} \delta [M \mu (\Delta w)]_j - \frac{1}{4} \delta [P \delta (\Delta w)]_j \\ &= - \sigma \delta(\mu f^n)_j + \frac{1}{2} \delta (Q \delta w^n)_j \end{aligned} \qquad (2)$$

where δ and μ are classical difference-operators in space defined by :

$$(\delta\psi)_j \equiv \psi_{j+\frac{1}{2}} - \psi_{j-\frac{1}{2}}$$

$$(\mu\psi)_j \equiv \frac{1}{2} (\psi_{j+\frac{1}{2}} + \psi_{j-\frac{1}{2}})$$

The general class of schemes (2) contains most of the explicit and implicit schemes used in practical applications (with centered or upwind space-differencing) including beside the 3-points schemes some second-order accurate TVD schemes. For predictor-corrector schemes, a

simple expression of the coefficients M, P and Q can be obtained (when system (1) possesses a strictly convex entropy) by using the Roe's linearization.

Properties of schemes (2) can be easily characterized in terms of their coefficients M, P and Q.

For instance, schemes (2) are second-order accurate in time and space if and only if :

$$Q(u, u, \ldots, u ; \sigma) = \sigma^2 [A^2(u) - M(u,u \ldots, u ; \sigma) A(u)]$$

for any $u \in \Omega$, where A(u) denotes the jacobian matrix of the flux f(u).

We shall determine the necessary and sufficient conditions for schemes (2) to be linearly stable and dissipative in the sense of Kreiss.

For explicit scalar approximations, we shall give the Tadmor's condition on Q to obtain the TVD property.

For implicit approximations, the schemes (2) lead to the solution of an algebraic linear system with a block-tridiagonal structure. The conditions to obtain solvability and diagonal dominance will be studied.

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An implicit centered scheme without artificial viscosity for the calculation of steady compressible flows with shocks

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Various time-dependent methods have been developed for the numerical solution of the Euler equations. In general, the space discretization is based on finite differences, finite volumes or finite elements, using either centered approximations or upwinding techniques. When second-order accuracy is required, space centered methods are simpler to implement but usually, they need the addition of some artificial viscosity term to damp spurious oscillations or even to stabilize the method, espacially in several space-dimensions.

For steady flow calculations, I plan to present an Euler solver of second-order accuracy which is linearly implicit and converges fastly to the steady-state. The original feature of the numerical method is to be centered in space and to give satisfactory results with no artificial viscosity. For multidimensional problems, the method does capture shock waves over one or two mesh cells without spurious oscillations. This means that the internal dissipation of the method is just sufficient to ensure the success of the calculation.

The implicit method is always linearly stable and it satisfies a property of diagonal dominance.

Applications to aerodynamic calculations will be described.

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Continuation methods for parameter-dependent boundary value problems

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ABSTRACT. An introduction is given into parameter-dependent nonlinear equations exhibiting nonuniqueness of solutions and bifurcation. In particular nonlinear systems of elliptic differential equations are considered. Recently proposed multigrid continuation methods are surveyed that have been implemented in public domain software. One area of application is the VLSI device simulation. Then related variational inequalities corresponding to obstacle problems are introduced. Theoretical results on continuation are quoted and a method is presented. Spurious transition points are observed in numerical computations.

1. Introduction
2. Nonlinear eigenvalue problems and bifurcation
3. Simple singular points
4. Nonlinear elliptic eigenvalue problems
5. Symmetry-breaking bifurcation
6. Continuation - two different approaches
7. Implementation
8. Application to VLSI - simplified prediction
9. Variational inequalities
10. Continuation for obstacle problems
11. Spurious transition points
12. Summary

Note: Only Ch. 1,2 reprinted here.

1. INTRODUCTION. Boundary value problems for partial differential equations that describe phenomena in different fields of application are usually nonlinear and depend on one or several parameters of the underlying system. With respect to these parameters frequently nonunicity effects and bifurcation occur. For a list of different problems from the applications as well as an introduction to analytic and numerical aspects see [18]. A survey of the state of the art was given in [15].

While parameter-dependent problems with known boundaries have been investigated recently by many researchers only little has been done so far for corresponding problems with a free boundary. Problems that can be written as parameter-dependent variational inequalities are the subject of [7,8,9,16,17,21,22,28].

Frequently, the only way to explore the solution manifolds of the above problems is to continue along the solution branches with respect to one or very few of the parameters for fixed values of the others. In the case of equations certain natural methods have been proposed and used for continuation (see [14,26,30]) while for variational inequalities both theoretical as well as numerical results were only obtained recently and these problems are still under investigation.

In the following we will survey some of the continuation methods proposed for both nonlinear equations and systems as well as variational inequalities. To make the presentation more self-contained some of the relevant theoretical results will be developed or quoted, too. For nonlinear systems of partial differential equations the emphasis will be on new continuation methods that have been implemented in public domain software. The field of applications includes in particular simulation of VLSI devices.

Many problems in mechanics and other engineering areas but also in other fields as, for example, mathematical economics have in addition to (initial) boundary conditions additional

constraints that often correspond to obstacles. The second part of this paper will deal with such problems. Theoretical results about continuation are given as well as an algorithm and some numerical results.

2. NONLINEAR EIGENVALUE PROBLEMS AND BIFURCATION. In this section a short presentation of some basic facts about the solutions of a general problem

$$(2.1) \qquad G(u,\lambda) = 0,\ G : X \times \mathbf{R} \to \mathbf{R}$$

will be given in order to provide some background and context for the following sections. X in (2.1) is some function space that will be specified later.

The general problem is to determine all (u,λ) that solve (2.1). Often solutions are sought that satisfy additional equations or conditions or that have certain properties. Of some importance are singular points (u_0,λ_0) of (2.1), i.e.

$$(2.2) \qquad G(u_0,\lambda_0) = 0, \qquad G_u(u_0,\lambda_0) \text{ singular.}$$

The simplest possible case is $X = \mathbf{R}$ and for this we give some very elementary examples.

Fold (turning) points

$$(2.3) \qquad G(u,\lambda) = Lu - \lambda e^u = 0,\ L \in \mathbf{R}$$

The singular point (cf. point A in Figure 2.1)

$$(u_0,\lambda_0) = (1,L/e)$$

is easily computed as is the graph of $G^{-1}(0)$. For each

λ, $0 < \lambda < \lambda_0$ there are two values of u. This nonuniqueness also implies by the implicit function theorem that

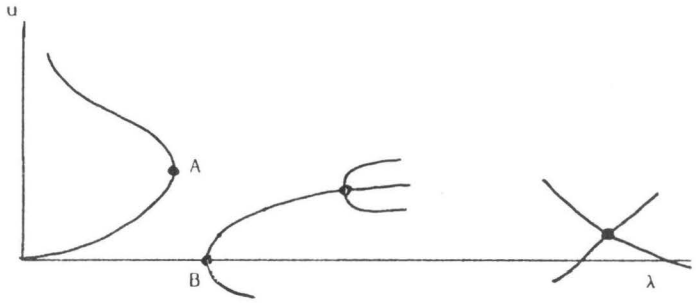

Fig 2.1. Bifurcation diagrams, singular points marked

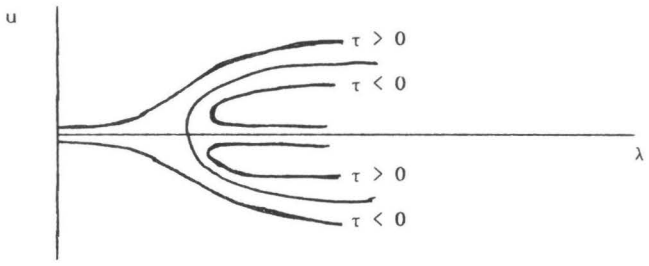

Fig 2.2. Perturbed bifurcation for (2.5)

G_u must be singular in (u_0, λ_0).

Bifurcation points

(2.4) $\quad G(u,\lambda) = Lu + cu^3 - \lambda u = 0,\ L,c \in \mathbf{R},\ c \neq 0$

There are two solutions

$$u^1(\lambda) = 0. \qquad u^2(\lambda) = \pm \sqrt{(\lambda - L)/c}\ .$$

The point $(u_0, \lambda_0) = (0, L)$ is a bifurcation point where the solution u^2 "branches" off u^1 (cf. point B in Figure 2.1).

Perturbed bifurcation

In general physical imperfections are present in the case that (2.1) describes a certain system. If on the other hand such a problem is approximated by, for example, discretization then errors are introduced. Both these phenomena effect the original problem in a similar way. This may be modeled for (2.4) by

$$G(u,\lambda) = Lu + cu^3 - \lambda u - \tau = 0, \quad \tau \in \mathbf{R} \tag{2.5}$$

where τ represents either an imperfection or an error term. It is again easy to see that the resulting bifurcation diagram is the one given in Figure 2.2.

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Weakly reflecting boundary conditions for external aerodynamic problems

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We consider problems governed by some set of first-order partial differential equations within a region Ω of space whose boundary is $\partial\Omega$, and an interval $[0,T]$ of time. When the p.d.e. is hyperbolic, the problem will be well-posed if data is completely specified over Ω at $t = 0$, and if the right sort of data is specified over $\partial\Omega$ for $t\in[0,T]$. Such initial-boundary-value problems can be very tricky, both at the differential and at the discrete level of description.

For problems in one space dimension the situation is fairly straightforward at the differential level. If the space domain is restricted to an interval $-1 < x < 0$, say, one may prescribe at each end of the domain as many variables as there are characteristics entering the domain. Moreover, for a well-posed problem, the prescribed data must not lie in the eigenspace of the outgoing waves [1]. Even given these constraints, however, the choice of boundary data for a given technological problem may not be straightforward. One must bear in mind Morretti's dictum that 'boundary conditions are a model for the rest of the universe'.

Often the problem of interest takes place in a domain that effectively extends to infinity. At the differential level one seeks to impose a 'radiation condition', that at large distances all energy flows outward. Computationally, such conditions have to be approximated at a finite distance. For some special cases, in which Riemann invariants exist [1], the connection between the boundary and infinity can be made analytically. There is then no loss of accuracy from placing the boundary at a finite distance.

In more general cases there are various ways of attempting to express mathematically the essentially negative statement that 'no disturbance originates outside the boundary'. The solution may be matched with some asymptotic form [2], or the boundary may be equipped with a memory [3]. Special far-field characteristic relationships have been derived [4].

The above considerations have to do with the physics of the real problem, and contribute nothing to solving the problems that arise at the discrete level due to the fact that many numerical methods permit high-frequency disturbances to propagate in a totally non-physical manner. For non-dissipative schemes an analysis of group velocity greatly clarifies these events [5,6]. High frequency wave packets can be shown to travel in the wrong direction. When they impact on a boundary, they reflect as low-frequency waves going the right way. Although the commonly-used Lax-Wendroff and Runge-Kutta methods are dissipative, and not covered by this analysis, the dissipation vanishes in the limit of small Courant number and high frequency (which are precisely the conditions applying at the outer edge of stretched grids). Numerical experiments close to this limit show the same anomalies found in non-dissipative schemes. For upwind schemes, the dissipation also vanishes in the same limit, but more rapidly, and this appears to eliminate the anomalous behaviour. It should be noted that these spurious effects can be triggered at internal boundaries also, ie. at places where the mesh density undergoes even a quite gradual change.

For multidimensional problems, there are additional difficulties. In principle, the number of variables that may be prescribed on the boundary can be determined from considering those terms in the p.d.e. arising from gradients normal to the boundary [7]. However, the accurate numerical description of the prescribed variables on the boundary of a reduced model of an infinite domain is made harder by the fact that the bicharacteristic equations contain exterior derivatives. Uncertainty about the correct conditions to be imposed often forces the use of very large computational domains. Intuitively, we may expect that accurate conditions would save computer space (smaller domains) and time (faster convergence). It may be necessary to take specific approaches that exploit the physics of each particular problem. In external aerodynamic problems, theorems of entropy and

vorticity give useful but incomplete information. Albone (private communication) obtains very accurate results on small grids by assuming power-law variation of certain 'Riemann variables'. The author has observed that a particular coordinate transformation enables the decay of pressure to be computed along specialised bicharacteristics in the mid-field [4]. These developments hold out the prospect for substantial reduction of computer costs.

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The numerical computation of bifurcation points arising in the finite Taylor problem

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This talk is concerned with the numerical calculation of bifurcating solutions of the Navier–Stokes equations for steady axisymmetric flow in the finite Taylor problem. In the Taylor problem the annular gap between two concentric circular cylinders is filled with a viscous fluid and it is the motion of this fluid that is studied. In our case the inner cylinder rotates with the outer one fixed. For this problem the phenomenon of bifurcation is intimately connected with the loss or gain of stability of the flows and this point will be discussed briefly.

In a recent series of papers Benjamin and Mullin (1978), (1981), and (1982), have carried out a theoretical and experimental study of the Taylor problem and have discovered an interesting variety of bifurcation phenomena. The apparatus has two parameters which may be adjusted, namely, the speed of the inner cylinder (in non–dimensional form, the Reynolds number, R) and the length of the annulus (in non–dimensional form, the aspect ratio, γ). A discrete model of this boundary value problem was obtained using a finite element method, and a medium–sized finite–dimensional nonlinear system

$$\underline{f}(\underline{x}, R, \gamma) = \underline{0} \quad (\underline{f} : \mathbb{R}^n \times \mathbb{R} \times \mathbb{R} \to \mathbb{R}^n)$$

was produced. Here n is in the range 2000–5000. There is a reflectional symmetry in the problem and it is important that this is preserved in the discretization. Thus, to summarise, we have a medium–sized, nonlinear, 2–parameter problem with a reflectional symmetry.

The numerical techniques are based on continuation, with bifurcation points computed using appropriate "extended" systems. The idea of extending (or enlarging) a system to compute a bifurcation point seems to have been first used by Seydel (1979) and Moore and Spence (1980). For example, the system

$$(\underline{f}, \underline{f}_x \underline{\phi}, \underline{\phi}^T \underline{\phi} - 1) = (\underline{0}, \underline{0}, 0)$$

has an isolated root $(\underline{x}, \underline{\phi}, \lambda)$ at a simple quadratic turning point and also at a symmetry breaking bifurcation point, provided $\underline{x}$ and $\underline{\phi}$ satisfy certain symmetry conditions (see Moore and Spence (1980) and Werner and Spence (1984)). The idea of extended systems can also be used to compute certain other "higher order" bifurcation points (see Spence and Werner (1982), and Jepson and Spence (1985)).

For problems of this size care must be exercised in handling the matrices that arise, though full advantage is taken of the software available at AERE Harwell where the calculations were performed. A direct method based on the frontal method (Duff (1984)) is used to produce LU factors of the matrices which arise in the discretization.

The numerical results were obtained using a CRAY–1S at AERE Harwell and some have been reported in Cliffe (1983) and Cliffe and Spence (1986).

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The use of singularity theory in the numerical analysis of bifurcation problems

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Multiparameter nonlinear problems mayexhibit an extensive variety of bifurcation phenomena, which can be extremely difficult to recognise and compute in most physical problems. The aim of this talk is to describe a strategy for the numerical solution of multiparameter problems based on some recent work in singularity theory by Golubitsky and Schaeffer (see their book referenced below, which was published in 1985, although their early work dates back to 1979).

Singularity theory provides a classification of bifurcation points which associates with each bifurcation point a system of equations and some inequalities, which together we call "defining conditions". The idea behind the numerical approach is to use standard continuation techniques in combination with these defining conditions to provide a variety of information, for example, regions in parameter space for which a problem exhibits the same type of bifurcation phenomena.

Many of the ideas have already been presented in Jepson and Spence (1985) for problems of the form

$$f(x, \lambda, \underline{\alpha}) = 0, \quad f : \mathbb{R} \times \mathbb{R} \times \mathbb{R}^P \rightarrow \mathbb{R}$$

Extensions to problems of the form

$$\underline{f}(\underline{x}, \lambda, \underline{\alpha}) = \underline{0}, \quad f : \mathbb{R}^n \times \mathbb{R} \times \mathbb{R}^P \rightarrow \mathbb{R}^n$$

were indicated in Jepson and Spence (1984) (compare with Beyn (1984)), and the talk will expand these ideas.

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Basic techniques in path following algorithms and applications to homotopy methods

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1. Let us given the underdetermined nonlinear system
$$F(y)=0, \quad F:R^{n+1} \to R^n, \ F \text{ smooth, rank } F'(y)=n, \qquad (1)$$
and let $y^0 \in L = \{y:F(y)=0\}$. Then the problem is to numerically follow the arc L^0 of L that contains y^0. Let $y^k \in L^0$ be the current iterate, and let v^k with $F'(y^k)v^k=0$, $\|v^k\|=1$ be the appropriately oriented tangent direction at y^k.
2. In order to find a successor y^{k+1} the path is locally parametrized by introducing the additional equation
$$N_k(y,\tau)=0, \quad N_k:R^{n+1}\times R \to R, \ N_k(y^k,0)=0 \qquad (2)$$
such that the inflated system (1),(2) has a locally unique solution $y=y_k(\tau)$ for small $|\tau|$. As examples, the generalized pseudo-arclength and the secant length parametrizations are discussed in detail. The successor is then defined by $y^{k+1}=y_k(\tau_k)$ with a certain stepsize τ_k.
3. Usually y^{k+1} is computed by a PC-method. At first, a predictor point $y^{k,0}$ is determined, and then $y^{k,0}$ is refined by applying a rapidly convergent method as Newton's method or some of its modifications to (1),(2) for $\tau = \tau_k$. Different corrector iterations are introduced, and a family of efficiently implementable higher order predictors is described.
4. The overall efficiency af a path following method strongly depends on the choice of stepsize. Some old and new stepsize algorithms are discussed and related complexity results are given.
5. In the corrector iteration, linear systems of a special bordered type are to be solved. Some methods for doing this are described which exploit properties as sparsity, bandedness, or symmetry.
6. In homotopy methods one has $y=(x,\lambda)$ with $x \in R^n$ and $\lambda \in R$, and the path is to be followed until the hyperplane $\lambda=1$ is crossed. This requires to adapt the usual methods to such a fixed parameter problem.

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Numerical methods for computing turning points of nonlinear equations

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1. We consider the underdetermined nonlinear System

$$F(y)=0, \quad F:R^{n+1} \to R^n, \ F \text{ smooth, rank } F'(y)=n \qquad (1)$$

that has the one-dimensional solution manifold $L = \{y:F(y)=0\}$. A point y^* on L is called a turning (or limit) point with respect to the e^{n+1}-axis if

$$e^{n+1T}v^* = 0 \quad \text{where } F'(y^*)v^*=0, \ \|v^*\|=1, \qquad (2)$$

i.e., v^* is the up to the sign unique tangent direction at y^*. The turning point is called a simple (or quadratic) turning point, if the λ-component $\lambda = e^{n+1T}y$ of the solutions y of (1) has a regular extremal value. This is equivalent to

$$e^{n+1T}\begin{pmatrix} F'(y^*) \\ v^{*T} \end{pmatrix}^{-1}\begin{pmatrix} F''(y^*)v^*v^* \\ 0 \end{pmatrix} \neq 0. \qquad (3)$$

In the following the conditions (2),(3) are assumed to be satisfied.

2. In the indirect turning point methods a local parametrization $y=y_k(\tau)$ of the path is used to construct a better approximation y^{k+1} to $y^* \in L$. A natural approach consists in interpolating $\lambda_k(\tau) = e^{n+1T}y_k(\tau)$ by a cubic polynomial $p_k(\tau)$ according to

$$\lambda_k(\tau_{k,j})=p_k(\tau_{k,j}), \ \dot{\lambda}_k(\tau_{k,j})=\dot{p}_k(\tau_{k,j}) \quad (j=k,k-1) \qquad (4)$$

at parameters $\tau_{k,j}$ which correspond to the last to points y^k, y^{k-1} on L. Then the smallest in modulus minimizer τ_k of $p_k(\tau)$ is taken as stepsize τ_k, and $y^{k+1}=y_k(\tau_k)$ is computed by a PC-method as solution of the system (1) inflated by the parametrizing equation. The method just described is Q-superlinearly convergent with R-order 2. Some other ways for defining τ_k are mentioned, too.

3. In the direct methods no parametrization is used but y^* is defined as solution of an extended system, e.g., of the system

$$F(y)=0, \ F'(y)v=0, \ e^{n+1T}v=0, \ r^Tv=1. \qquad (5)$$

At a simple turning point this system has a regular Jacobian, and Newton's method converges Q-quadratically. It is also possible to eliminate $v=v(y,r)$ from the equations $F'(y)v=0$, $r^Tv=1$ which leads to the reduced system

$$F(y)=0, \ e^{n+1T}v(y,r)=0 \qquad (6)$$

only in y. Applying Newton's method to (5) or (6) requires to compute the terms $F''(y)vv$ and $F''(y)vs$. In order to avoid the explicit use of second derivatives efficient difference approximations to these terms are proposed.

4. Direct methods can be used to compute curves of turning points in two parameter problems. Special techniques are avaiable for computing cusps on those curves.

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On numerical methods for invariant curves

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In this paper we consider a map Φ from $\mathbb{R}^d$ to $\mathbb{R}^d$, such that $\Phi\gamma \subset \gamma$ for a simple closed curve γ. In many instances this map Φ is the Poincaré map (return map) of a differential equation. The invariant curve γ may represent a manifold with quasi-periodic solutions, or a heteroclinic orbit, or, in $\mathbb{R}^2$, the boundary of a domain of attraction of a fixed point of Φ. Nice examples may be found in Koçak[2], both for differential equations and difference equations.

We discuss simple algorithms based on the work of Kevrekides et al.[1]. The limitations of these algorithms will be discussed, cf.[3], and convergence results wil be given, cf.[4]. Some results for the delayed logistic map and the Van der Pol equation wil be given.

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[3] Veldhuizen, M. van: A New Algorithm for the Numerical Approximation of an Invariant Curve. To appear in SIAM J. Sci. Stat. Comp.

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A numerical study of nonlinear wave-interactions in bubbly two-phase flow

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Abstract

The derivation of macroscopic equations which govern the two-phase flow of a bubbly liquid/gas mixture leads to a model with complex characteristics when important physical aspects are not included.
It has been shown that virtual mass can be used to derive a macroscopic model with real characteristics and that this model may be extended to include the effect of flow induced bubble-deformation (J.A. Geurst, Physica 129A (1985) 233 and J.A. Geurst, A.J.N. Vreenegoor, Proceedings ICIAM '87 335).
The models allow two types of waves, void-fraction waves and pressure waves.
The LUSMD scheme which consists of a hybrid combination of a scheme introduced by Lerat and a minimum dispersion scheme (P. wilders, thesis, Univ. of Amsterdam, 1984) is used to investigate numerically the nonlinear interaction of the two kinds of waves.
The calculations show that void-fraction waves are stable in the sense that they recover after interference with a pressure wave.
Moreover it is shown that pressure waves can be partially reflected, partially transmitted during their interaction with a void-fraction wave.
Since only slight modifications were needed to change the program solving the first model (four PDE's) into a program solving the extended model (five PDE's) the LUSMD scheme turned out to be very useful.

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