CONFERENTIE VAN NUMERIEK WISKUNDIGEN

29,30 september en 1 oktober 1980

CONFERENTIEOORD WOUDSCHOTEN
ZEIST

Werkgemeenschap Numerieke Wiskunde

VIJFDE CONFERENTIE NUMERIEKE WISKUNDE

Uitgave verzorgd door het
MATHEMATISCH CENTRUM
AMSTERDAM

DOEL VAN DE CONFERENTIE

Het doel van de conferentie is hen die betrokken zijn bij onderzoek en/of onderwijs in de numerieke wiskunde de gelegenheid te geven kennis te nemen van de stand van zaken op enkele gebieden van de numerieke wiskunde en de gelegenheid te geven met elkaar en met buitenlandse sprekers intensief van gedachte te wisselen.

THEMA

De thema's zijn:

- Snelle oplosmethoden voor elliptische differentiaalvergelijkingen.
- Randwaardeproblemen met vrije of bewegende randen.

ORGANISATIE

De organisatie is in handen van de voorbereidingscommissie bestaande uit de heren van de Vooren (RUG), Slagt (MC), Veltkamp (THE) en Wesseling (THD), en van het Mathematisch Centrum.

SPREKERS

J. CARA, INRIA, le Chesnay, France.

J. CRANK, Brunel University, Uxbridge, UK.

G.H. GOLUB, Stanford University, U.S.A.

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J.R. OCKENDON, Oxford University, U.K.

U. SCHUMANN, Kernforschungzentrum, Karlsruhe, BRD.

Bovendien hebben 2 deelnemers zich bereid verklaard in een korte bijdrage een schets van hun onderzoek op het gebied van het conferentiethema te geven, t.w.

J.W. BOERSTOEL, Nat.Lucht- en Ruimtevaartlab., Amsterdam.

P. WESSELING, Technische Hogeschool, Delft.

PROGRAMMA

Maandag 29 september

10.00-11.15	aankomst en koffie	15.15-15.45	thee
11.15-12.30	opening, Golub	15.45-16.45	Henrici
12.45	lunch	16.50-17.15	Boerstoel
14.15-15.15	Crank	17.20-18.00	Wesseling
		18.10	diner

dinsdag 30 september

8.00	ontbijt	12.45	lunch
9.00 -10.00	Cara	15.15-15.45	thee
10.00-10.30	koffie	15.45-16.45	Crank
10.30-11.30	Schumann	16.50-17.50	Golub
11.35-12.35	Ockendon	18.00	diner

woensdag 1 oktober

8.00	ontbijt	12.45	lunch
9.00 -10.00	Ockendon	13.45-14.45	Henrici
10.00-10.30	koffie	14.45	sluiting, thee
10.30-11.30	Cara		vertrek
11.35-12.35	Schumann		

TITELS EN SAMENVATTINGEN VOORDRACHTEN

Monday, 29 september

11.15 opening

G.H. Golub: Some direct methods for solving separable equations.

14.15 J. Crank: How to deal with moving boundaries in thermal problems.

15.45 P. Henrici: Fast Fourier methods for Poisson's equation in a rectangle (the point of view of the numerical analyst).

16.50 J.W. Boerstoel: On the application of a multigrid approach in flow calculations.

17.20 P. Wesseling: Some remarks on multigrid methods.

Tuesday, 30 september

9.00 J. Cara: Numerical solution of vortex ring problems I.

10.30 U. Schumann: Cyclic reduction and influence matrix techniques for fluid-structure-interaction simulations.

11.35 J.R. Ockendon: Free and moving boundary problems in heat flow and diffusion.

15.45 J. Crank: Solution of free boundary problems by variable interchange.

16.50 G.H. Golub: Solutions by the conjugate gradient method of sparse systems of linear equations arising from partial differential equations.

Wednesday, 1 october

9.00 J.R. Ockendon: Calculation of weak solutions of free and moving boundary problems.

10.30 J. Cara: Numerical solution of vortex ring problems II.

11.35 U. Schumann: Numerical solution of elliptic equations on domains with periodic structure.

13.45 P. Henrici: Fast Fourier methods for Poisson's equation in a rectangle (the point of view of the mathematical physicist).

HOW TO DEAL WITH MOVING BOUNDARIES IN THERMAL PROBLEMS

John Crank, Brunel University, Uxbridge, England.

Moving boundary problems in heat flow have been widely studied in recent years from both numerical and analytic points of view. Much of the interest has been stimulated by the need to solve practical problems in science and engineering. Reports on three recent conferences (Ockendon & Hodgkins, 1975; Wilson et al, 1978; Furzeland, 1979) give good impressions of the present state of the art and extensive lists of references to previous and current work. Other up to date surveys are given by Furzeland (1977), Hoffmann (1977), Fox (1979) and Crank (1980), all with useful bibliographies.

This paper concentrates mainly on methods of obtaining numerical solutions which have been applied to two or three dimensional problems and on approaches to one-dimensional problems which are promising for extension to higher dimensions or problems complicated in other ways.

A moving boundary problem or Stefan problem is taken to mean a time-dependent problem presented by a parabolic partial differential equation together with a prescribed initial condition and boundary conditions, two of which are given on a boundary or boundaries which move in a way that depends on the solution of the partial differential equation. Heat conduction or diffusion problems with phase changes constitute a large class of moving boundary problems.

A simple version of the original moving boundary problem studied by Stefan round about 1890 is the melting of a semi-infinite sheet of ice, initially at zero temperature (the melting temperature) throughout, the surface of which is raised at time $t = 0$ to a constant temperature, above zero, at which it is subsequently maintained. A boundary or interface on which melting occurs moves from the surface into the sheet and separates a region of water from a region of ice at zero temperature.

If $u(x,t)$ denotes the temperature distribution in the water phase and $X(t)$ the position of the interface, both at time t, the problem is to find both these unknowns by solving the heat flow equation, in non-dimensional terms,

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \quad , \quad 0 < x < X(t), \quad t > 0 \quad , \tag{1}$$

subject to a fixed boundary condition

$$u = 1 \quad , \quad x = 0 \quad , \quad t > 0 \quad , \tag{2}$$

and initial conditions

$$u = 0 \quad , \quad x > 0 \quad , \quad t = 0 \quad , \tag{3}$$

$$X(0) = 0 \quad . \tag{4}$$

Two conditions are needed on the moving boundary, the second in order to find its position at any time. For melting ice they are

$$\left.\begin{aligned} u &= 0 \qquad\qquad (5) \\ \frac{\partial u}{\partial x} &= -\frac{dX(t)}{dt} \qquad (6) \end{aligned}\right\} \quad x = X(t) \quad , \; t > 0 \quad .$$

A few very limited analytic solutions are available for simple problems such as the two-phase melting problem in a semi-infinite medium, due to Neumann (see Carslaw and Jaeger, 1959; Crank, 1975).

Goodman (1961) assumed a temperature profile for each phase, e.g. a quadratic form, and reduced a set of integral equations obtained by integrating the heat flow equations with respect to the space variable to a set of ordinary differential equations in time which yield the velocity of the moving boundary. Noble (in Ockendon & Hodgkins,1975, p.208) and Bell (1978) have suggested introduction of finite elements so that the integral method is applied within each element. Poots (1962) and Poots & Rodgers (1976) have extended the heat balance method to two space dimensions and Imber and Huang (1973) have included temperature-dependent thermal properties.

Boley (in Ockendon 1975, p.150) has applied his embedding techniques to the melting of a solid in one space dimension, when the liquid is instantaneously removed on formation.

Other analytic techniques are outlined by Ockendon and Hodgkins (1975) and Furzeland (1977) including an integral-equation formulation by Hansen and Hougaard (1974) and asymptotic expansions and perturbation methods.

Numerical methods can be classified conveniently under four headings.

(i) Front-tracking methods

In a one-dimensional problem the moving boundary at any time will usually lie between two points or nodes on the finite-difference or finite-element grid. Modified finite-difference formulae based on unequal intervals near the boundary (Crank, 1957; Saitoh, 1972) are needed to track the motion of the boundary in successive time steps. Ehrlich (1958) and Koh et al (1969) used Taylor expansions in time and space near the moving boundary. Furzeland (1977) reviews various ways of front tracking. Irregular grids in two and three space dimensions were used by Lazaridis (1970). Murray and Landis (1959) used space grids adjusted in size at each time step so that the number of space intervals between the fixed and moving boundary in a one-dimensional problem remained constant and the partial differential equation was modified accordingly. Miller et al (1978) use elements of standard length for most of the space range and adopt only the two elements nearest the moving boundary. Bonnerot and Jamet (1974, 1975, 1977, 1979) and Jamet (1978) have used variable finite elements in one and two space dimensions.

Meyer (1975, 1976, 1977, 1977a, 1978) has developed extensively the method of lines in which only the time variable is discretised and the partial differential equation is replaced by a sequence of ordinary differential equations at successive time levels.

(ii) Front-fixing methods

In one space dimension various authors - Landau (1950), Crank (1957), Ferriss and Hill (1974) - have fixed the moving boundary for all times by a coordinate transformation, e.g. $\xi = x/X(t)$ fixes the boundary $x = X(t)$ at $\xi = 1$ for all time, t. This transformation is a simple example of the general use of curvilinear coordinates and Furzeland (1977a), Saitoh (1978) and Sparrow et al (1978) have used a transformation in two dimensions due to Oberkampf (1976) analagous to that of Murray and Landis (1959). Further applications are discussed by Hoffmann (1977), Vol. III.

(iii) Isotherm migration method

A particular curvilinear transformation is defined by interchanging the dependent variable, temperature u, with one or other of the space variables, e.g. we calculate $x = x(u,t)$ instead of $u = u(x,t)$. If the moving boundary is an isotherm this transformation fixes the boundary in the (u,t) plane.

Because the change in the position x of an isotherm u is calculated, it is called the isotherm migration method (IMM). Crank and Phahle (1973) have used an IMM in one space dimension and Crank and Gupta (1975), Crank and Crowley (1978, 1979) extended it to two-dimensional problems.

(iv) Enthalpy and other fixed domain methods

Some problems can be reformulated in a way that avoids the need to solve two partial differential equations, one in each phase of a two-phase problem for example, with their solutions coupled through the conditions on the melting interface.

One procedure is to introduce an enthalpy function, $H(u)$, where $H(u)$ is the sum of the specific heat and latent heat contents. We then solve a single differential equation

$$\rho \frac{\partial H}{\partial t} = \frac{\partial}{\partial x}\left(K \frac{\partial u}{\partial x}\right) ,$$

where ρ (density) and K may be functions of temperature, u, over the whole of a fixed domain in the original physical plane.

The essential feature is that the interface effectively disappears from the process of numerical solution and its position is obtained, a posteriori, from the values of the space coordinate(s) where $u = u_M$ = the melting temperature. The enthalpy method has been used by Eyres et al (1946), Albasiny (1956), Atthey (1974), Comini et al (1974), Meyer (1976), Furzeland (1977a) and in two space dimensions by Crowley (1978).

Elliott (1976) demonstrated links between discretisations of the enthalpy formulation and discretised forms based on variational inequalities which lead to a quadratic programming problem of minimisation at each time level. Elliott and Janovsky (1977) extended the method to more than one space dimension. The truncation method of Berger et al (1975, 1975a, 1976) is loosely related.

Duvaut (1973, 1975) has based a variational inequality formulation on the Baiocchi transformation (1972).

References to theoretical studies of weak solutions by Brezis (1972) and others are given in Furzeland (1977).

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SOLUTION OF FREE BOUNDARY PROBLEMS BY VARIABLE INTERCHANGE

John Crank, Brunel University, Uxbridge, England.

The most extensively studied free-boundary problem refers to the seepage of water through an earth dam which separates a high reservoir from a lower one. The free boundary is the upper surface of the water within the dam and the position and shape of this surface have to be determined as part of the solution.

Successive authors have approached this and other problems by solving a sequence of fixed boundary problems corresponding to successive, iteratively-computed positions of the free boundary. Relaxation methods, finite differences and finite elements have all been used to execute the solution. Key references are to be found in Cryer (1976), Aitchison (1972, 1977) and Furzeland (1977, 1979).

More recently, Aitchison (1977), Elliott (1978, 1980) and others referred to in Furzeland (1977, 1979) have avoided the iterations by using the Baiocchi transformation (1972), to reformulate the problem as a variational inequality over a fixed domain.

In another class of methods the region within the dam contained partly by the free boundary is transformed by some change of variables into a new domain with fixed, known boundaries. The hodograph method (Bear, 1972) is one example.

The present paper describes a special case of a curvilinear transformation in which the dependent variable, representing potential, is interchanged with one of the independent space variables. This idea is well tried in potential flow problems and has recently been applied to moving boundary problems in heat flow (Crank and Phahle, 1973; Crank and Gupta, 1975; Crank and Crowley, 1978, 1979). A closely similar, though on the face of it a numerically more cumbersome, method in which the three space variables x, y, z are interchanged with the three velocities u, v, w, is described by Jeppson (1972). One method based on such a variable interchange is applied to the rectangular dam problem in two dimensions by Crank and Ozis (1980). The mathematical formulation in terms of the velocity potential $\phi(x,y)$ calls for a solution of Laplace's equation for ϕ ,

$\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} = 0$, subject to two conditions on the free boundary,

$\phi = y$ and $\partial\phi/\partial n = 0$, where n is the outward normal.

Crank and Ozis interchange the variables ϕ and x in the term $\partial^2\phi/\partial x^2$ and write $x(\phi,y)$ as the new dependent variable. Laplace's equation becomes

$$\frac{\partial^2\phi}{\partial y^2} - \frac{\partial^2 x}{\partial \phi^2}\left(\frac{\partial x}{\partial \phi}\right)^{-3} = 0 ,$$

and the conditions on the free boundary are now

$$g' + \left(\frac{\partial x}{\partial y}\right)_{\phi} = 0 , \quad y = \phi ,$$

where $g' = dy/dx$ along the free boundary. They compute values of $x(\phi,y)$ on a finite-difference grid subject to Cauchy or Neumann conditions on the other boundaries in the (ϕ,y) plane. The free boundary becomes the line $y = \phi$ in the new plane. Crank and Ozis (1980) obtain values for $(\partial^2\phi/\partial y^2)_x$ at the point $(i\delta\phi, j\delta y)$ in the new (ϕ,y) plane by using interpolated values of ϕ on the lines $y = y_{j-1}$, $y = y_j$ and $y = y_{j+1}$ at the three points for which $x = x_{i,j}$.

The so-called "separation point" at which the free surface joins the down-stream face of the dam is known to lie on the line $y = \phi$ in the transformed plane but its location on the line has to be determined. Crank and Ozis use an iterative algorithm which approximates within each single loop both a finite-difference solution of the transformed partial differential equation $x(\phi,y)$ and the position of the free boundary $x(y) = x(\phi)$, including the location of the separation point.

More recently, Crank and Sabouri-Shojai (1980) have made a complete transformation of Laplace's equation following Boadway (1976), including the term $\partial^2\phi/\partial y^2$. The same iterative treatment of the resulting system of finite-difference equations yields more accurate results for the dam problem with fewer iterations than the interpolative treatment of $\partial^2\phi/\partial y^2$ used by Crank and Ozis.

The latter authors have also considered a dam in the form of a quadrant of a cylindrical annulus, both as a radially-symmetrical problem in two space dimensions (r,z) and also as a model three-dimensional problem in cartesian coordinates (x,y,z). Their method of interchanging the dependent variable ϕ with the vertical space variable z, so that the free surface becomes the plane $\phi = z$, is found to work in three space dimensions.

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SOME DIRECT METHODS FOR SOLVING SEPARABLE EQUATIONS

by

Gene H. Golub

Abstract

For many elliptic partial differential equations for which the method of separation of variables is applicable, it is possible to construct numerical procedures which take advantage of this property. In particular, consider the problem of solving the finite difference approximation to Poisson's equation

(1) $$\Delta u = f \quad \text{in} \quad R$$
$$u = g \quad \text{on} \quad \partial R$$

where R is a rectangular region. The finite difference approximation to (1) leads to a system of linear algebraic equations

$$\underset{\sim}{A}\underset{\sim}{x} = \underset{\sim}{b} .$$

The matrix A is a symmetric block tri-diagonal matrix; all blocks are symmetric and commute with one another. These properties allow for two basic methods:

(1) matrix decomposition,

(2) cyclic reduction.

A third procedure is a combination of the two methods.

In this talk, we shall give the derivation to a variety of problems. We shall also discuss the situation when the method of separation of variables is not applicable but for a "nearby" problem the method of separation of variables can be applied; we are thus led to the capacitance matrix approach.

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SOLUTION BY THE CONJUGATE GRADIENT METHOD OF SPARSE SYSTEMS OF LINEAR EQUATIONS ARISING FROM PARTIAL DIFFERENTIAL EQUATIONS

by

Gene H. Golub

Abstract

We consider the problem of solving the system of linear algebraic equations

(1) $$\underset{\sim}{A}\underset{\sim}{x} = \underset{\sim}{b}$$

where A is a real $n \times n$ matrix and b is a given vector. It is frequently possible to rewrite the system (1) in the form

(2) $$\underset{\sim}{M}\underset{\sim}{x} = \underset{\sim}{N}\underset{\sim}{x} + \underset{\sim}{c}$$

where M is a symmetric, positive definite matrix. We discuss the following situation:

(3.a) $N = N^T$, N is symmetric;

(3.b) $N = -N^T$, N is skew-symmetric;

(3.c) $N = N^T$ and $\text{rank}(N) = p$ with $p \ll n$.

For matrix problems satisfying (2) and any of the conditions (3.a) (3.b) or (3.c) the conjugate gradient (cg) method is a very effective technique providing it is "easy" to solve the system of equations

(4) $$\underset{\sim}{M}\underset{\sim}{z} = \underset{\sim}{d}\ .$$

We shall derive the cg method algebraically and show how it may be viewed as an acceleration method.

For some problems, the matrix M and N have the following structure:

$$M = \begin{pmatrix} M_1 & 0 \\ 0 & M_2 \end{pmatrix} , \qquad N = \begin{pmatrix} 0 & F \\ F^T & 0 \end{pmatrix}$$

and thus

$$M^{-1} N = \begin{pmatrix} 0 & M_1^{-1}F \\ M_2^{-1}F^T & 0 \end{pmatrix} . \tag{4}$$

Matrices with the structure given by (4) are said to possess "Property A." This structure arises in solving Poisson's equation by finite differences over regions which are T-shaped and problems with interfaces. We shall show how the conjugate gradient method may be modified to simply the calculation when $M^{-1}N$ has Property A. We shall also report the result of various numerical experiments where the conjugate gradient method has been used with matrix splittings.

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Conference on Numerical Analysis, September 29 - October 1, 1980, Woudschoten, the Netherlands

Abstract of talks by P. Henrici (Zurich), "Fast Fourier methods for Poisson's equation in a rectangle".

Part A: The point of view of the numerical analyst. In the present context, a numerical analyst by definition is a person who solves Poisson's equation $-\Delta u = f$ either by the method of finite differences or by a version of the finite element method. If finite differences are used, it is either possible to approximate $-\Delta$ at any mesh point by a (more or less accurate) finite difference approximation or, more sophisticatedly, to use a "Mehrstellenverfahren" of a type first proposed by Collatz, which approximates $-\Delta u = f$ only at the desired solution, but there more accurately, and which results in an expression of the form $Du_{ij} = Ff_{ij}$, where both D and F are finite difference operators. Similar finite difference approximations also result if the finite element method is used. If the region under consideration is a rectangle, if the boundary conditions are such that the solution may be continued periodically, and if standard finite difference approximations are used, it has been known since Hockney that the resulting equations may be solved by finite Fourier techniques, which via the Fast Fourier Transform results in very efficient solution algorithms. It is the main point of this lecture that this approach works for arbitrary difference operators, also of the Mehrstellen type and also for those obtained from the

finite element method; even more general differential operators with constant coefficients may be considered. To this end we present a short account of the discrete Fourier transform in several dimensions. It will then be seen that the operators D and F introduced above can be viewed as convolutions, which by taking Fourier transforms are converted into ordinary Hadamard products. This observation immediately leads to simple solution algorithms for the discrete solution u_{ij} in the general case.

Part B: The point of view of the mathematical physicist. Here a mathematical physicist by definition is a person who solves $-\Delta u = f$ by means of eigenfunction expansions. If, for the region under consideration, the eigenfunctions u_n and the eigenvalues λ_n of the operator $-\Delta$ are known, the solution of $-\Delta u = f$ can be written in the form $u = \Sigma\, (a_n/\lambda_n)u_n$, where the a_n are the Fourier coefficients of f. If the region is a rectangle, both the eigenfunctions and the eigenvalues are known explicitly, and thus a fairly explicit formula for the exact solution is available. Its numerical implementation again requires discrete Fourier methods; however, full advantage may now be taken of known numerical techniques for dealing with Fourier series, such as Gautschi's attenuation factors. In particular, any knowledge of the degree of smoothness of the solution may be taken into account. It thus seems that the method of the mathematical physicist is more flexible and thus, in principle, preferable. This confirms the results of Sköllermo. Something may be saved, however, for the purposes of nume-

rical analysis. It turns out that the ratio of the Fourier transforms of the operators D and E introduced in part A are approximations, in a certain sense, to the eigenvalues λ_n introduced above. We may cross this bridge in the opposite direction and, from rational approximations to λ_n obtained by means of multi-dimensional Padé techniques, construct accurate finite difference approximations for $-\Delta u = f$, both of the conventional and of the Mehrstellen type. These difference approximations can then be used for arbitrary regions. The order of convergence as the mesh tends to zero can, for smooth solutions u, be read off directly from the degree of approximation to λ_n.

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Free and Moving Boundary Problems in Heat Flow and Diffusion

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We will begin by describing the classical Stefan problem [1] which is the most famous moving boundary problem in heat flow. It is an idealised model for heat conduction in a pure substance in which a phase change occurs at a prescribed temperature. The points at which the phase change occurs are unknown a priori and comprise the "moving boundary". Modifications will be given to the classical model to account for the effects of internal heating [2], variable thermal properties [3] and the diffusion of an impurity [4,5,6], but many other important real phenomena will be ignored. In particular we will not discuss the convective effects which always occur when a density change accompanies the phase change [7]. Analogies will be drawn with other problems in mass transfer, in particular the "oxygen-consumption" problem [8] and the problem of percolation of a vapour in a porous medium [9].

A Stefan problem is called a "one-phase" problem when one of the two phases present is everywhere at the phase change temperature, assumed constant. When the specific heat is much smaller than the latent heat, the two-dimensional one-phase Stefan problem will be shown to be equivalent to the "Hele-Shaw" problem [10] of the flow of a liquid blob between two parallel plates whose distance apart is small compared to the size of the blob. Experimental observations will be made of such a flow and analogies will be drawn between the Hele-Shaw problem and problems of flow in porous media [11], electro-chemical machining [12], lubrication theory [13] and crystal growth [14]. A very brief review will be given of the use of complex variable theory to obtain explicit solutions to some of these problems [15].

Calculation of weak solutions of free and moving boundary problems

The classical Stefan problem will be reformulated as a conservation law in terms of the "enthalpy" or heat content. This will motivate the definition of the weak solution to the Stefan problem [16] . An outline will be given of the proof of convergence of the solution of certain discretisations of the enthalpy formulation to the weak solution [2, 17] . The principal advantage of these discretisations is that the moving boundary does not have to be tracked explicitly but it simply emerges as the locus of points at which the temperature is the phase change temperature. Hence the method is called a "fixed domain" method. The possibility of extending the idea of fixed domain methods to the generalised Stefan problems described earlier will be discussed and some open questions will be posed [6] . In particular, it is an interesting question as to which moving boundary problems are amenable to fixed domain methods, so we will briefly contrast the enthalpy method to some other methods of this type [18, 19, 20, 21] .

We will conclude with a brief discussion of so-called "unstable" moving boundary problems as typefied by the classical Stefan problem when the latent heat is negative. It is known that even in one space dimension the solution can become singular in finite time [22] and in two or more space dimensions, short wavelength oscillations in the moving boundary will grow rapidly [23] . The way in which this behaviour is reflected in fixed domain numerical methods will be discussed and the question will be posed as to how such problems might be "smoothed" to obtain physically sensible results.

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CYCLIC REDUCTION AND INFLUENCE MATRIX TECHNIQUES FOR FLUID-STRUCTURE-INTERACTION SIMULATIONS

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Abstract

The lecture covers three parts, a description of a particular fast elliptic solver, the influence matrix technique, and an application of these methods to a nuclear reactor safety analysis problem.

1) We start with a description of a special fast elliptic solver for solution of the linear system of equation $\underline{\underline{L}}\,\underline{u} = \underline{v}$ where the matrix $\underline{\underline{L}}$ is N x N block-tridiagonal:

$$\underline{\underline{L}} = \begin{bmatrix} (A-\alpha I) & -I & & & \\ -I & A & -I & & \\ & & \ldots & & \\ & & -I & A & -I \\ & & & -I & (A-\beta I) \end{bmatrix}$$

$$A = \begin{bmatrix} b_1 & c_1 & & & a_1 \\ a_2 & b_2 & c_2 & & \\ & & \ldots & & \\ & & & & \\ c_M & & & a_M & b_M \end{bmatrix}$$

Here, I = M x M unit matrix, a_i, b_i, c_i are scalars, $|b_i| \geq |a_i| + |c_i|$, $i = 1, 2, \ldots, M$. Such systems arise if certain elliptic equations are discretized, e.g. by finite differences. Here $\alpha,\beta = 0$ appears for Dirichlet and $\alpha,\beta = 1$ for Neumann boundary conditions. The solution method requires an order MN log N operations. The method is based on cyclic reduction. Unlike the original Buneman version of this alorithm the present scheme is not restricted to specific values of N or M but any value $N \geq 2$, $M \geq 2$ can be taken. The method is fully described in [1, 2, 3], related methods are described in [4 - 9]. The method is available as a FORTRAN or PL/1 program.

2) Fast solution methods, like the described elliptic solver, generally require a particularly structured linear system. If a given linear system has a matrix which differs from the matrix of a fast solvable one in a few rows only then the influence matrix technique can be employed to set up an efficient solution scheme. In the literature this technique is commonly termed "capacitance matrix technique", however this name does not cover its great generality. A short summary of the influence matrix technique [10, 11, 3] will be given.

3) The above methods are applied in an implicit integration scheme of the three-dimensional pressure wave equation coupled with elastic walls. The scheme simulates the pressure loadings on nuclear reactor vessel internal structures after a sudden break of one of the coolant inlet pipes [12]. The application demonstrates that fast solution schemes can indeed be applied with advantage for complicated technical cases.

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NUMERICAL SOLUTION OF ELLIPTIC EQUATIONS ON DOMAINS WITH PERIODIC STRUCTURE

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Abstract

In this lecture exact and approximate solution methods are described for large discretized elliptic equations in a domain with periodic structure.

Such problems appear, for example, in the analysis of composites like fiber enforced materials, of plates with a periodic pattern of holes, or of a rod bundle immersed in a fluid. Often one does not want or cannot solve the relevant continuum equations on such domains in all details. Rather one sets up "homogenized" continuum models which have smooth solutions. Such homogenization methods are described, e.g., in [1-5]. In such theories, at the final stage of analysis, a solution of the local differential equations is required on a single characteristic cell of the domain. Usually one has to setup a discretization and a numerical solution scheme at this stage.

Here the local differential equations are discretized from the beginning on the whole domain. Of course the number of unknowns envolved is huge. Nevertheless, for cases with periodic boundary conditions at the boundaries of the total domain, these equations can be solved rather efficiently employing Fast Fourier Transform. Moreover, there is a pendant to homogenization for the discrete problem: one can reduce the number of unknowns per cell by using a proper transformation. The main discussion of this lecture concentrates on the question how this "discrete homogenization" has to be done so that for certain restrictions the approximation error is a minimum. No references on this question have been found in the literature.

In two dimensions, the discrete set of equations under discussion can be written in the form

$$\sum_{i=-1}^{1} \sum_{i=-1}^{1} \underline{\underline{A}}_{i,j}\ \underline{u}(m_1+i,\ m_2+j) = \underline{v}(m_1,\ m_2) \qquad (1)$$

$$\dim\ (\underline{u}\ (m_1,\ m_2)) = n,$$

$$m_1 = 0,1,\ldots,N_1-1;\quad m_2 = 0,1,\ldots,N_2-1$$

(index expressions are to be taken modulo N_1 or N_2.)

Here m_1, m_2 are the indices of the $N_1 \times N_2$ cells which form the domain. The vectors $\underline{u}(m_1,\ m_2)$ and $\underline{v}(m_1,\ m_2)$ contain the n unknowns or right-hand-sides (r.h.s.) related to the cell $(m_1,\ m_2)$. Because of the periodic cell configuration, the matrices $\underline{\underline{A}}_{i,j}$ are independent of m_1 and m_2.

The goal is to reduce the system to a much smaller one

$$\sum_{i=-1}^{1} \sum_{j=-1}^{1} \hat{\underline{\underline{A}}}_{i,j}\ \hat{\underline{u}}(m_1+i,\ m_2+j) = \hat{\underline{v}}(m_1,\ m_2), \qquad (2)$$

$$\dim\ (\underline{u}\,(m_1,\ m_2)) = m \ll n$$

$$m_1 = 0,1,\ldots,N_1-1;\ m_2 = 0,1,\ldots,N_2-1$$

so that

$$\tilde{\underline{u}}(m_1,\ m_2) = \underline{\underline{E}}\ \hat{\underline{u}}(m_1,\ m_2) \qquad (3)$$

gives a least squares approximation to $\underline{u}$, i.e. the error

$$\delta^2 := \sum_{m_1=0}^{N_1-1} \sum_{m_2=0}^{N_2-1} |\underline{u}(m_1,\ m_2) - \tilde{\underline{u}}(m_1,\ m_2)|^2 \qquad (4)$$

should become a minimum for fixed $m \ll n$ and given r.h.s.

It will be shown that under certain smoothness-conditions the minimum is obtained if *)

$$\hat{\underline{\underline{A}}}_{i,j} = \underline{\underline{E}}^{*} \underline{\underline{A}}_{i,j} \underline{\underline{E}}; \quad i = -1,0,1; \quad j = -1,0,1;$$

$$\hat{\underline{v}}(m_1, m_2) = \underline{\underline{E}}^{*} \underline{v}(m_1, m_2); \; m_1 = 0,\ldots,N_1-1; \quad m_2 = 0,\ldots,N_2-1; \tag{5}$$

and if $\underline{\underline{E}}$ is composed of the first eigenvectors $\underline{x}_k$ of the local eigenvalue-problem"

$$\left\{ \sum_{i=-1}^{1} \sum_{j=-1}^{1} \underline{\underline{A}}_{i,j} \right\} \underline{x}_k = \lambda_k \underline{x}_k, \quad k = 1,2,\ldots,n. \tag{6}$$

Here, the ordering of the eigensolutions must be taken such that

$$|\hat{v}_k/\lambda_k|^2 \leq |\hat{v}_{k+1}/\lambda_{k+1}|^2, \quad k = 1,2,..,n-1 \tag{7}$$

where

$$\hat{v}_k = \sum_{m_1=0}^{N_1-1} \sum_{m_2=0}^{N_2-1} \underline{x}_k^{*} \underline{v}(m_1, m_2). \tag{8}$$

The equation (2) are termed the "discretely homogenized equations". We will see, that the smoothness requirements are essentially the same as those assumed in "continously" homogenized models.

Our discussion also applies to periodic systems which are discrete itself, like crystal lattices [6].

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*) The star denotes the conjugate complex transposed quantity.

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