Mausam, (1985), **36**, 4, 441-446

551.465:551.510.62

A review of computational techniques in flow network models*

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(*Received 2 April 1981*)

सार – इस शोध पत्र में प्रवाह संजाल समस्याओं के संगणक अनुरूपण में उपयोगी कई संगणकीय एल्गोरिथ्मों पर विचार विमर्श किया गया है। इस पत्र में दीर्घ संरचना वाली समस्याओं से निबटान के लिये सटीक, तीव्र तथा कम लागत वाली तकनीकों पर जोर दिया गया है। अवनिर्धारित समस्याओं के मामलों में आसान बनाने वाली तथा संबंधित तकनीकों का क्रिया-वयन, जो वांछित समाधान प्रस्तुत करेगा, उसका वर्णन किया गया है। समाधान प्रक्रिया में संगणक भण्डारण तथा चलाने के समय में कमी करने के लिये निदर्श संरचना का कैसे उपयोग किया गया है। यह इसमें दिखाया गया है। प्रदत्त प्रणाली की बिखराव वाली संरचना को छोड़े बिना स्पलाइनों के उपयोग से आंकिक योजनाओं की सटीकता को कैसे सुधारा गया, इस पर भी इस पत्र में चर्चा हुई है।

ABSTRACT. Several computational algorithms which have been found useful in the computer simulation of flow network problems are discussed. The emphasis is on accurate, fast and low-cost methods for handling large structured problems. In the case of underdetermined problems, the implementation of smoothing and related techniques that yield a class of desirable solutions is described. It is shown how the model structure has been utilized in the solution process to save computer storage and run time. How the accuracy of the numerical schemes has been improved by the use of splines without disturbing the sparsity structure of the given system is also discussed.

1. Introduction

The flow network problems consist of a set of tubes which interact transmurally with a common environment while the direct tubal flow outputs of some tubes are the inputs for others. The mathematical models of such flow networks require the numerical solution of a system of highly coupled stiff differential equations with multipoint-boundary conditions. Shooting methods for the solution cannot be used due to the intricate connectivity of the tubes and the environment and, therefore, global finite difference techniques have to be used. In most cases this requires the solution of large systems of non-linear algebraic equations. However in order to achieve a realistic computer simulation of a given flow network, it is necessary to have fast and accurate methods which lead to small discretization errors and require the solution of non-linear equations of reasonable size.

In many cases, due to experimental constraints enough information about the model is not available. For example, one can only sample at the end points of the interval of interest, or cost and hardware make it impossible to get enough data as in satellite remote sensing, picture reconstruction, oil exploration. In these cases the problem is under-determined. If it is known that the desired solution is smooth, then we can use the Sobolev type norms in the solution process to obtain unique solutions.

In the next section, we describe a simple model and the related differential and algebraic equations. In Section 3, computational methods are given. These methods make efficient use of the model structure in the solution process. The given set of equations is partitioned into the so-called *basic* and *non-basic* variables and equations. Using the non-basic equations, the non-basic variables are expressed as functions of the basic variables. These values of non-basic variables are then substituted in the basic equations and this procedure results in the basic equations being expressed as functions of only the basic variables. Gaussian elimination, Implicit Function Theorem or Quasi-Newton type methods are then used to compute the Jacobian of the basic equations as functions of basic variables.

The partitioning of the equations and variables into basic and non-basic sets is done by proper ordering of tubes and the compartments within each tube. The order is usually determined by the direction of flow. Generally speaking, the environment (also called the bath) and some other critical tube variables and equations are taken as basic.

*The paper was presented in the symposium "Indo-French School on Recent Advances in Computer Techniques in Meteorology, Biomechanics and Applied systems', held at Indian Institute of Technology, New Delhi, 4-13 February 1980.

The whole model can then be expressed in terms of these basic equations and variables. The net result of this transformation is that the basic equations are solved less often than the non-basic ones. In the case of flow network problems, connectivity matrices of the non-linear algebraic equations resulting from box difference schemes which use the Trapezoidal Rule are of doubly bordered, overlapping, block diagonal forms. The non-basic equations and variables correspond to the overlapping block diagonal forms and the basic variables and equations are associated with the borders. Clearly, the solution of basic equations for basic variables is easy.

In addition to making use of the model structure in the solution process, we also need high accuracy in the finite difference approximations. Very small step sizes are ruled out since they lead to unwieldy algebraic equations. Therefore, it is shown in Section 4 that instead of the Trapezoidal Rule, higher order methods like the corrected Trapezoidal Rule, Cubic and Fifth degree overhang, can be used. The use of these leads to higher connectivity in the algebraic equations. This is handled by using a deferred correction type approach; the terms leading to additional connectivity are moved to the right hand side and then an iterative scheme is used. We have found recently that highly accurate Euler-Maolaurin type integration formulas can be used if the derivative terms are computed by using splines. The increase in connectivity is handled as indicated above.

Finally, in the last section, we will review some methods that make use of spline programs to determine smoothing matrices which are then used to impose the necessary smoothing restrictions on the solutions of underdetermined problems.

2. A simple flow network

Let us consider the network shown in Fig. 1 (Pinter & Shohet 1963 etc). Fluid enters under pressure at the tops of tubes 1 and 3 after flowing in the directions indicated by arrows in the figure exits from the top of tube 2 and the bottom of tube 3. The bath, which is labelled 4, has an overflow so that its volume remains constant. The walls of the tubes are semi-permeable and therefore some part of the solvent and some of the solutes permeate and/or are pumped in or out of the tubes to the common bath.

Let us define the following :

x : normalized distance measured from the top of the bath ($x=0$ at the top; $x=1$ at the bottom)

For $i=1, 2, 3, 4$ and $p=1, 2, 3, 4$

$y_{ip}(x)$: axial flow, $p\neq 4$,

: pressure if $p=4$.

$f_{ip}(x)$: transmural flux

$\underline{y}(x) = \left(y_{ip}(x) \right)$: vector with $y_{ip}(x)$ as components.

Then the differential equations are

$$\frac{dy_{ip}(x)}{dx} = f_{ip}\left(x, \underline{y}(x) \right) \tag{2.1}$$

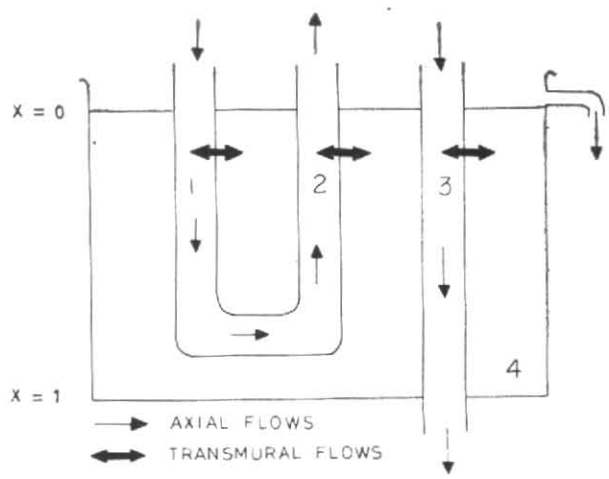

Fig. 1. A simple flow network

with the two point boundary conditions

$$L\left(\underline{y}(0), \underline{y}(1) \right) = 0 \tag{2.2}$$

where L is usually a linear operator. The transmural fluxes are connected by the equations

$$\sum_{i=1}^{3} f_{ip}(x) + f_{4p}(x) = 0 \tag{2.3}$$

The above equation and (2.1) can be used to replace the differential equations for the bath by the algebraic equations

$$\sum_{i=1}^{3} y'_{ip}(x) + y'_{4p}(x) = 0,$$

which on integration yield

$$\sum_{i=1}^{3} y_{ip}(x) + y_{4p}(x) = \text{constant}. \tag{2.3a}$$

In order to solve (2.1) we first let

$$h = 1/n,\ x_j = h_j,\ j = 0, 1, 2, \ldots\ldots, n,$$

$$y_{ipj} = y_{ip}(x_j) \quad \text{and} \quad f_{ipj} = f_{ip}\left(x_j, \underline{y}(x_j) \right),$$

then for $p\neq 4$, integrate (2.1) to get

$$y_{ipj} - y_{ip,\,j-1} - \int_{x_{j-1}}^{x_j} f_{ip}\left(x, \underline{y}(x) \right) dx = 0. \tag{2.4}$$

If the integrand in the above equation is evaluated by the well known Trapezoidal Rule (TR) and we let

$$\phi_{ipj} = y_{ipj} - y_{ip,\,j-1} - (h/2)(f_{ipj} + f_{ip,j-1}),\ p \neq 4, \tag{2.5}$$

then in view of the fact the TR has an $0(h^3)$ error, we have

$$\phi_{ipj} + 0(h^3) = 0,\ p\neq 4, j = 1, 2, \ldots, n \tag{2.6}$$

Now from (2.3a) it follows that

$$\sum_{i=1}^{3} y_{ipj} + y_{4pj} = \text{constant}.$$

If we let

$$\phi_{4pj} = \sum_{i=1}^{3} (y_{ipj} - y_{ip,j-1}) + y_{4pj} - y_{4p,j-1} \tag{2.7}$$

then evidently

$$\phi_{4pj} = 0 \quad . \tag{2.8}$$

Since L is linear, some of the variables y_{ipo} and/or y_{ipn} are either given explicitly or as functions of the other variables. This leads to only as many variables y_{ipj} as there are Eqns. in (2.6) and (2.8), *viz.*, $16n$ for the model under consideration.

Now if we let

$$\underline{\alpha} = (y_{ipj}),\ \underline{\theta} = (\phi_{ipj}),\ i \neq 4,$$

$$\underline{\beta} = (y_{4pj}),\ \underline{\psi} = (\phi_{4pj}),$$

then neglecting the $0(h^3)$ term we can write (2.6) and (2.8) as

$$\underline{\theta}(\underline{\alpha}, \underline{\beta}) = 0 \tag{2.9a}$$

$$\underline{\psi}(\underline{\alpha}, \underline{\beta}) = 0 \tag{2.9b}$$

In the next section we describe the implementation of Newton's method for the solution of (2.9). This method has turned out to be the best of a large class of problems (Stephenson *et al.* 1974 etc).

3. Computational considerations

It turns out that $\underline{\theta}(\underline{\alpha}, \underline{\beta}) = 0$ is easy to solve for $\underline{\alpha}$ for a given value of $\underline{\beta}$ because due to the structure of flow network models $\dfrac{\partial \underline{\theta}}{\partial \underline{\alpha}}$ is an overlapping block diagonal matrix, then we can write $\underline{\alpha} = T(\underline{\beta})$, such that $\underline{\theta}(T(\underline{\beta}), \underline{\beta}) = 0$.

Substituting this in (2.9b), we have

$$\underline{\psi}(T(\underline{\beta}), \underline{\beta}) = 0 \tag{3.1}$$

and this is now solved as a function of only $\underline{\beta}$. One can use the Gausian elimination, Implicit function theorem or a quasi-Newton method to solve (3.1) (Juang 1976 etc). The use of these methods has led to great savings in computer costs and made it possible to have comprehensive and realistic simulation of renal concentrating mechanism. Convergence and uniqueness properties of models of this type are discussed (Kellogg 1975 etc).

The partitioning of variables and equations on the basis of complexity and model structure is useful in many diverse modelling situations.

Large systems are broken down into a number of small components for conceptual and modelling purposes. In most cases, it is physically impossible for each component to interact with all the others, as the following examples show: in a large company the head office interacts with each branch office but the latter interact with only a few others; in an ecosystem each species interacts with a common environment but with only a few other species; in hierarchical systems, each component reports to and is instructed by the next level of command.

In each of the cases mentioned above, it is easy to ascertain the component which basically determines the whole system. The variables and equations associated with these components are called critical, *basic*, important, sensitive, global or leaders, bosses, trouble markers, etc. The remaining variables and equations are labelled non-critical, *non-basic*, unimportant, dependent, local or workers, followers, etc.

In some systems it is not easy to determine the basic components. In such cases, graph theoretic methods that include the model structure or numerical methods using the domain of attraction and convergence rate can be used to determine a basic set of components.

The determination of basic variables and equations is very closely related to the following practical questions. Where to make a finer grid and/or make more accurate measurements when studying the global interaction of air currents, temperature and pressure for weather forecasting? What are the critical finite elements so that disection methods can be used in designing bridges and other structures? How to find the points of attachment for partitioning and tearing electrical and other network? What are the critical areas in diffusion and transport problems (water purification, renal modelling, nuclear reactor simulation, etc) ?

The separation of the variables and equations into the 'basic' and 'non-basic' categories has been called decomposition, splitting, partitioning, tearing, disection and/or modification.

For example, according the Rheinboldt (1975):

". . . in the analysis and design of electrical networks physical considerations usually allow a decomposition of a large network into smaller components; in large-scale control problems multilevel approaches are often introduced; and in linear or non-linear programming, decomposition techniques have long been the key to the solution of surprisingly large-scale problems."

"When no effective decomposition is found, that is, when one or more of the subsets of equations is still at large, it is often possible to gain some improvement by a tearing approach."

"Tearing by inspection is often performed in practical applications. For example, large structural problems are usually broken down into sub-problems and so-called super-elements are introduced which model the behaviour of separately analyzed components."

Applications of decomposition techniques in electrical network, heirarchical and multigoal systems environmental problems, linear and nonlinear programming are discussed in detail in (Himmelbau 1973), where, among other things, Himmelbau observes in the preface:

"Probably the fundamental underlying idea that evolved at the conference was that a large complex system representing interacting elements could be broken down into sub-problems of lower dimensionality."

On page 4, in discussing 'structure and sparseness', he writes :

"Tewarson (1971) illustrated a number of structures (the occurrence matrices) for A, that might be obtained by partitioning or permutation, and would generate a minimum number of new non-zero elements during the forward phase of the elimination".

Robertson (1976), in connection with the numerical solution of stiff ordinary differential equations, observes:

". . . if the slower variables were at any time clamped (*i.e.,* held fixed), the fast responding variables would quickly tend towards and remain at equilibrium values. System of equations having these properties arise in a variety of applications, including chemical reaction kinetics, particularly where very reactive intermediate species are produced, guidance and control problems, electrical transmission networks, and heat and matter transfer."

An excellent survey of

"... preordering techniques ... with particular emphasis on partitioning (to block triangular form) and tearing (to bordered triangular form)."
is given by Duff (1976).

Steward observes that partitioning and the tearing approach of the precedence matrix is the basis for organizing engineering work. Steward's method for tearing is described in Tewarson (1977). Sargent (1977) gives an algorithm for decomposing large-scale computing problems which have a network structure and sparse systems of algebraic equations.

Partitioning and tearing is the subject of the following papers:

Bunch and Rose (1974) :

"The computational complexity of partitioning sparse matrices is developed graph theoretically. The results are used to study tearing and modification ... arithmetic and memory costs are considered."

Tarjan (1976), where two graph theoretic partitioning methods are given.

Duff and Reid (1976) :

".....an implementation of an algorithm of Tarjan (1972) for symmetrically permuting a given matrix to block triangular form".

Bunch (1976), where

"Graph-theoretic techniques for analysing the solution of large sparse systems of linear equations by partitioning and block methods....."

are developed.

Sangiovanni-Vincentelli (1976), which has a heuristic algorithm for getting a (bordered) lower triangular form. More recent work on this topic is given in Nepomiastchy (1978), where the border variables are called 'loop' variables.

Cheung and Kuh (1974), where

".... the problem of transforming a non-singular matrix by symmetric permutation to an optimal bordered triangular form....."

is solved. Additional comments on this paper and some uses are given in Kevorkian (1976) and the determination of numerically stable pivots is described in Kevorkian (1976).

Disection, splitting and modification are described in the following papers :

: Birkhoff and George (1973), where it is shown by an example how reordering can make it a doubly bordered block diagonal form and

".....a precise recommendation for the choice of disection sets for George's (1973) nested disection ....."

is given. Furthermore,

".....experimental comparisons with the minimal degree algorithm of Markowitz (1957)."
are also given.

Concus *et al.* (1978) where it is shown how to

".....split the original discretized operator into the sum of two operators, one of which corresponds to a more easily solvable system of equations, and accelerate the associated iteration based on this splitting by (nonlinear) conjugate gradients".

and to make use of the Block Successive Over-relaxation and Cholesky factorization in algorithms which approximate the Jacobian by an operator that is computationally easier to invert.

Stone (1968), Buzbee (1976), Tuff and Jennings (1973), Jennings (1977) and Kershaw (1978), where the easy part is factorized once and for all and iteration is used to take care of the difficult part.

Most of the above mentioned papers do cite examples or mention the applications of sparse nonlinear equations. Some additional examples are given in Porsching (1976), where a variety of source problems which give rise to sparse nonlinear equations are mentioned. Applications in computational circuit design and partial differential equations are given (Rose & Willoughby 1972). Computer aided network analysis and design is discussed by Hachtel *et al.* (1971). Equilibrium flows in a network are mentioned (Porsching 1969).

4. Methods of higher accuracy

Instead of the Trapezoidal Rule, higher order integration formulae can be used in (2.4) to

evaluate $\int_{x_{j-1}}^{x_j} f_{ip}\left(x, y(x)\right) dx$. These lead to smaller errors but with some decrease in the sparsity of $\partial\underline{\theta}/\partial\underline{\alpha}$. We first briefly describe some of these schemes and then show how a deferred correction type approach can be used to overcome the sparsity decrease (Tewarson 1978). Let us drop the subscripts i and p, and let

$$I = \int_{x_{j-1}}^{x_j} f\left(x, \underline{y}(x)\right) dx$$

then we have the following :

(a) *Corrected Trapezoidal Rule*

$$I = \frac{h}{2}(f_j + f_{j-1}) - \frac{h^2}{12}(f'_j - f'_{j-1}) + 0(h^5).$$

(b) *Cubic overhang method*

$$I = \frac{h}{24}(-f_{j-2} + 13f_{j-1} + 13f_j - f_{j+1}) + 0(h^5).$$

(c) *Simpson's Rule*

$$I = \frac{h}{6}(f_j + 4f_{j-\frac{1}{2}} + f_{j-1}) + 0(h^5).$$

Hermite interpolation on y_j, y_{j-1}, y'_j, and y'_{j-1} is used to get $y_{j-1/2}$, which is then used to compute $f_{j-1/2}$

(d) *Quintic overhang method*

I is a function of f_{j-k} ; $k = -3, -2, -1, 0, 1, 2,$ and the errors are $0(h^7)$.

(e) *Euler-Maclaurin type formulae*

$$I = \frac{h}{2}(f_j + f_{j-1}) - \frac{h^2}{10}(f'_j - f'_{j-1}) - \frac{h^3}{120}(f''_j + f''_{j-1}) + 0(h^7).$$

The derivatives f' and f'' can be computed by cubic or quintic slines or directly by differentiating f.

(f) *Optimum formulae using the y and f values*

One such formula is

$$\sum_{p=-1}^{2} (a_{j+p}\, y_{j+p} - b_{j+p}\, f_{j+1}) = 0.$$

The coefficients a_{j+p} and b_{j+p} are chosen to such that $y' = f$ and Taylor's theorem lead to the least error, *viz*; $0(h^6)$.

There is no change in the structure of $\frac{\partial\underline{\theta}}{\partial\underline{\alpha}}$ when (a) or (c) replace the Trapezoidal Rule. On the other hand the, use of (b), (d), (e) and (f) leads to significant decrease in the sparsity of $\frac{\partial\underline{\theta}}{\partial\underline{\alpha}}$. This can be alleviated by writing $\underline{\theta} = \underline{\theta}_{TR} + \underline{\theta}_C$ and using $\frac{\partial\underline{\theta}_{TR}}{\partial\underline{\alpha}}$ in place of $\frac{\partial\underline{\theta}}{\partial\underline{\alpha}}$. This slows down the convergence but under proper conditions, which are usually fulfilled in practice, converges reasonably fast (Tewarson 1979.) In view of the above facts, evidently the methods described in the last section for the Trapezoidal Rule can be used with advantage. Computational experimentation has shown this to be the case.

5. Use of splines to compute smoothing matrices

In many cases the system of nonlinear algebraic equations (2.9) may be underdetermined and/or only smooth solutions are of interest (Tewarson 1977). Then we have to solve $\underline{\phi}(\underline{y}) = 0$ with the constraint that $y^T W y$ is a minimum, where W is a smoothing matrix associated with a Sobolev norm of the type

$$||y||_W^2 = \sum_{v=0}^{2} \sum_{j=1}^{n} \left|\frac{d^v y}{dx^v}\right|^2 x = x_j \qquad (5\cdot1)$$

The W matrix can be computed efficiently by the spline routines as follows (Tewarson 1979)

The spline programs have f_j as input and f'_j as the initial computational result.

Thus

$$\underline{f}' = B\underline{f} + 0(h^4) \qquad (5.2)$$

where $\underline{f}' = (f'_j)$ and $\underline{f} = (f_j)$.

The matrix B can be easily determined from the program since

$$B = \frac{d\underline{f}'}{d\underline{f}}$$

The second derivative is computed by a spline on spline program and therefore

$$\underline{f}'' = B\underline{f}' = B^2\underline{f} + 0(h^3). \qquad (5.3)$$

It follows from (5.1)–(5.3) that

$$W = I + B^T B + B^{2T} B^2 + 0(h^2),$$

and if quintic-splines are used then the error is of $0(h^3)$.

In this paper we have given a brief review of various computational techniques that have been found useful in solving large scale flow network problems that arise mainly in renal modelling. Most of these techniques have been used on test problems in the published literature from other areas with excellent results. The overall aim in modelling large systems is to be able to get fast and accurate soutions without an inordinate expenditure of computing time and storage. We have attempted to show some of the recent efforts made to achieve this aim.

Acknowledgements

The author would like to thank Professor M.P. Singh, IIT, Delhi, India for inviting him to the Indo-French School; Dr. J.L. Stephenson and Mr. R. Mejia of the National Institutes of Health, Bethesda, MD; and Professor R.B. Kellogg of the University of Maryland for their continued interest and support. The author's past and present doctoral students : Dr. A. Kydes, Dr. L.L. Juang, Dr. A. Tsan, Dr. P. Farahzad, Mr. D. Salane, Mrs. Y. Shraga, Ms. Y. Nakai and Mr. C. Song for their enthusiasm and collaboration.

This research was supported by NIH Grant No. 2 RO 1 AM17593-04A2. The air travel of the author was supported by NSF travel grant INT 8002303.

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