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A Hybrid Numerical-Analytical Method for the Solution of Partial Differential Equations in Ground-Water Modelling

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Abstract

Many numerical problems in ground-water modelling deal with the solution of differential equations of the form

$$\delta u/\delta t = D_x (u)$$

where D_x is a differential operator in the space coordinates, but which is invariant in time. If D_x can be approximated by a finite expression involving values of u at nodal points of a finite difference grid, for example, we obtain a set of n ordinary differential equations

$$du_i/dt = \mathbf{A}u_i + c_i, \quad i=1,n$$

where n is the number of nodes at which u is evaluated, and **A** is an n x n matrix of constant coefficients. This set of equations can be solved as

$$u_i = \sum_{j=1}^{n} b_{i,j} e^{\lambda_j t}, \qquad i=1,n$$

or

$$u = Be^{\lambda_j t}$$

where the λ_j are the eigenvalues of A and the columns of matrix B are the eigenvectors of A.

Résumé

De nombreux problèmes numériques en modélisation des eaux souterraines exigent la solution d'équations différentielles de la forme :

$$\delta u/\delta t = D_x\ (u)$$

où D_x est un opérateur différentiel selon les coordonnées spatiales, mais invariant dans le temps. Si D_x peut être approché par une expression finie faisant intervenir des valeurs de u à des noeuds d'une grille de différences finies, par exemple, on obtient un ensemble de n équations différentielles ordinaires :

$$du_i/dt = \mathbf{A}u_i + c_i, \quad i=1,n$$

où n est le nombre de noeuds où u est évalué, et **A** est une matrice n x n de coefficients constants. Cet ensemble d'équations possède la solution suivante :

$$u_i = \sum_{j=1}^{n} b_{i,j}\, e^{\lambda_j t}, \qquad i=1,n$$

ou

$$u = \mathbf{B}e^{\lambda_j t}$$

où les λ_j sont les valeurs propres de A et les colonnes de la matrice B, les vecteurs propres de A.

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INTRODUCTION

In standard finite difference and finite element procedures for the solution of differential equations, both the time derivative $\delta u/\delta t$ as well as the space derivatives are approximated by a finite expression, resulting in a set of n equations, one for each of n locations in the space domain defined by the boundary conditions. These equations can then be solved simultaneously or explicitly for the values of u at one time step, Δt, following the time for which the initial condition is given at first, and thereafter at a time step, Δt, following the time of the previous solution. Since for an accurate solution the time steps must be kept rather small, a large number of steps will often be required even though the solution may be needed only at one point in time. It is, however, possible to find a solution that is continuous in time and discrete only in the space coordinates by approximating the space derivatives in terms of finite differences, but leaving the time derivative in its infinitesimal form. It will be shown how the resulting set of simultaneous differential equations can be solved giving u_i, the value of u at all the n locations, as an analytical function of time. For ease of presentation, the method will be demonstrated for a set of only three locations. The general equations for n nodes will then be given in matrix notation, and finally the method will be illustrated by a three-point problem.

THE HYBRID METHOD

Although the method can be applied to any linear partial differential equation, the discussion will be based on the parabolic equation in two-dimensional space

$$\partial u/\partial t = \alpha \partial^2 u/\partial x^2 + \beta \partial^2 u/\partial y^2 + \gamma \tag{1}$$

where the α, β, and γ are invariant with time.

In the hybrid method, Equation 1 is replaced by an approximate form, for example,

$$\partial u_{i,j}/\partial t = (\alpha_{i,j}/\Delta x^2)(u_{i-1,j} - 2u_{i,j} + u_{i+1,j})$$

$$+ (\beta_{i,j}/\Delta y^2)(u_{i,j-1} - 2u_{i,j} + u_{i,j+1}) + \gamma_{i,j} \tag{2}$$

The subscripts i and j indicate that the values of u, α, β, and γ are the values at the intersections of the ith north-south line and the jth east-west line of a regular grid, with spacings of Δx in the east-west direction and Δy in the north-south direction (Fig. 1).

Writing out Equation 2 once for each of the nodes (i,j) results in the set of ordinary differential equations

$$\begin{aligned} du_1/dt &= a_{11}\, u_1 + a_{12}\, u_2 + a_{13}\, u_3 + c_1 \\ du_2/dt &= a_{21}\, u_1 + a_{22}\, u_2 + a_{23}\, u_3 + c_2 \\ du_3/dt &= a_{31}\, u_1 + a_{32}\, u_2 + a_{33}\, u_3 + c_3 \end{aligned} \tag{3}$$

or in matrix notation

$$du/dt = \mathbf{A}u + c \tag{4}$$

where **A** is the matrix

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

and c is a vector of constants, deriving in part from the constants γ in Equation 1 and partially from constant values of u on the boundaries of the domain of definition of u, as will be shown in the example. The

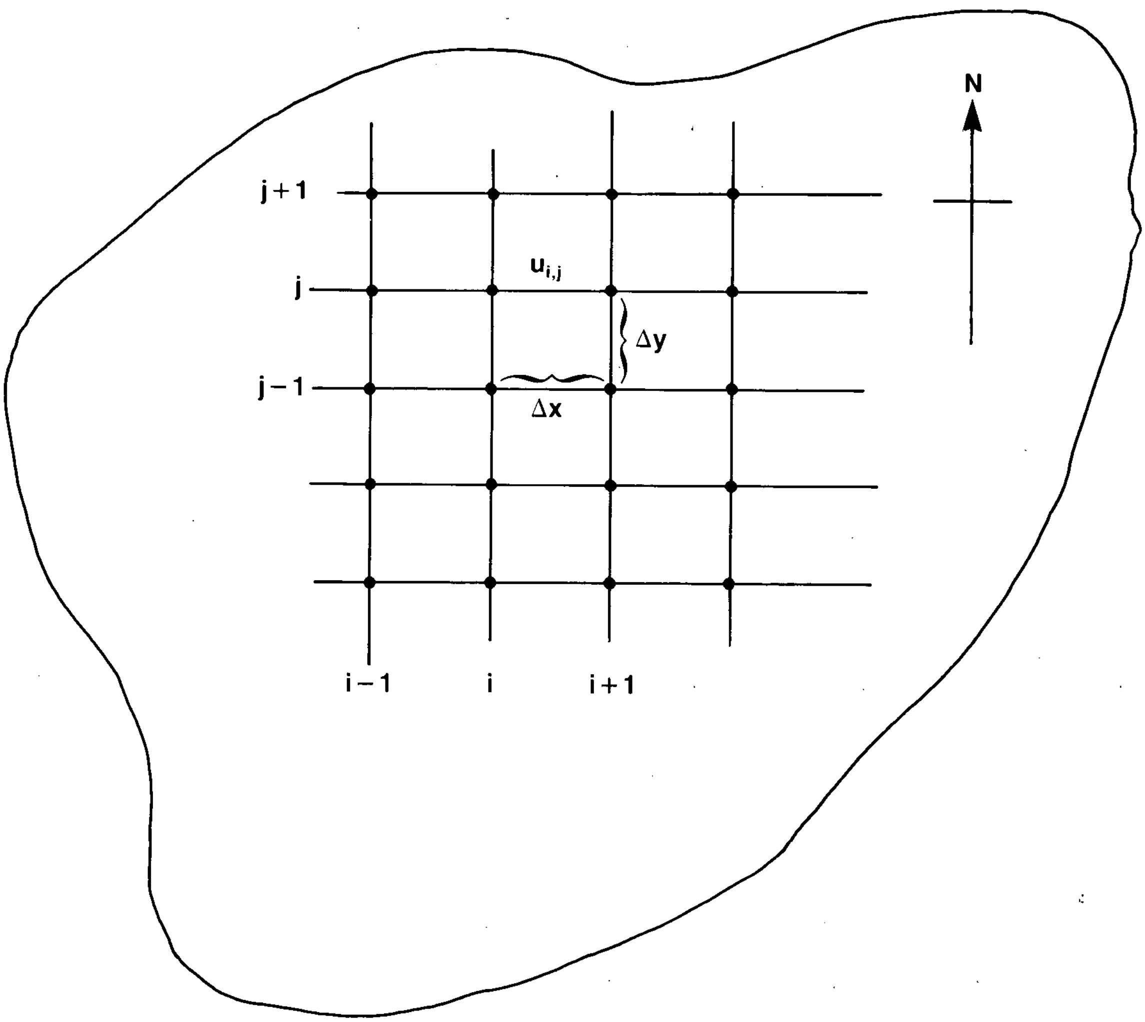

Figure 1. Notation used in the finite difference approximation.

boundary conditions, which are an integral part of the problem, are thus already contained in Equations 3 and 4, but a set of initial conditions must be defined:

$$u_i \ (t=0) = u_{oi} \tag{5}$$

It will now be shown that a solution to the set of ordinary differential equations (4), subject to the initial conditions (5), exists, which has the form

$$u_1 = b_{\infty 1} + b_{11} \ e^{\lambda_1 t} + b_{12} \ e^{\lambda_2 t} + b_{13} \ e^{\lambda_3 t}$$

$$u_2 = b_{\infty 2} + b_{21} \ e^{\lambda_1 t} + b_{22} \ e^{\lambda_2 t} + b_{23} \ e^{\lambda_3 t}$$

$$u_3 = b_{\infty 3} + b_{31} \ e^{\lambda_1 t} + b_{32} \ e^{\lambda_2 t} + b_{33} \ e^{\lambda_3 t}$$

or in matrix notation

$$u = b_{\infty} + Be^{\lambda t} \tag{6}$$

where $e^{\lambda t}$ represents the vector

$$e^{\lambda_1 t}, \ e^{\lambda_2 t} \ \ldots \ e^{\lambda_n t}$$

Note that if the system is to reach a steady state for $t \to \infty$, then all λ must be negative, and the vector b_{∞} thus represents the steady state at each of the n nodes. Also, from Equation 4, at steady state,

$du/dt \to 0$, and since $u \to b_\infty$, we have

$$Ab_\infty + c = 0$$

or

$$b_\infty = -A^{-1}c \tag{7}$$

where A^{-1} is the inverse of A.

When Equation 6 is evaluated at t=0, we obtain the relations

$$\begin{aligned} u_{01} &= b_{\infty 1} + b_{11} + b_{12} + b_{13} \\ u_{02} &= b_{\infty 2} + b_{21} + b_{22} + b_{23} \\ u_{03} &= b_{\infty 3} + b_{31} + b_{32} + b_{33} \end{aligned} \tag{8}$$

which will be used later on to completely define the matrix B.

In order to find the vector λ and the matrix B, Equation 6 is differentiated:

$$du_1/dt = b_{11}\,\lambda_1\,e^{\lambda_1 t} + b_{12}\,\lambda_2\,e^{\lambda_2 t} + b_{13}\,\lambda_3\,e^{\lambda_3 t}$$

$$du_2/dt = b_{21}\,\lambda_1\,e^{\lambda_1 t} + b_{22}\,\lambda_2\,e^{\lambda_2 t} + b_{23}\,\lambda_3\,e^{\lambda_3 t}$$

$$du_3/dt = b_{31}\,\lambda_1\,e^{\lambda_1 t} + b_{32}\,\lambda_2\,e^{\lambda_2 t} + b_{33}\,\lambda_3\,e^{\lambda_3 t}$$

or

$$du/dt = B\lambda e^{\lambda t} \tag{9}$$

where $\lambda e^{\lambda t}$ is the vector $\lambda_i e^{\lambda_i t}$, i=1,n.

Combining Equations 9, 4, and 6 gives

$$\mathbf{A}u + c = \mathbf{B}\lambda e^{\lambda t}$$

and

$$\mathbf{A}(b_\infty + \mathbf{B}e^{\lambda t}) + c = \mathbf{B}\lambda e^{\lambda t} \tag{10}$$

which must hold for all values of t.

At very large t, and given that all λ must be negative, we find

$$\mathbf{A}b_\infty + c = 0$$

which result was already obtained earlier.

Therefore Equation 10 can be rewritten

$$\mathbf{AB}e^{\lambda t} = \mathbf{B}\lambda e^{\lambda t} \tag{11}$$

The elements $(ab)_{i,j}$ of the matrix **AB** are given by

$$(ab)_{i,j} = \sum_{k=1}^{n} a_{ik}\, b_{kj}$$

and we have from Equation 11:

$$(ab)_{11}\, e^{\lambda_1 t} + (ab)_{12}\, e^{\lambda_2 t} + (ab)_{13}\, e^{\lambda_3 t} = b_{11}\,\lambda_1\, e^{\lambda_1 t} + b_{12}\,\lambda_2\, e^{\lambda_2 t} + b_{13}\,\lambda_3\, e^{\lambda_3 t} \tag{12}$$

$$(ab)_{21}\, e^{\lambda_1 t} + (ab)_{22}\, e^{\lambda_2 t} + (ab)_{23}\, e^{\lambda_3 t} = b_{21}\,\lambda_1\, e^{\lambda_1 t} + b_{22}\,\lambda_2\, e^{\lambda_2 t} + b_{23}\,\lambda_3\, e^{\lambda_3 t} \tag{13}$$

$$(ab)_{31}\, e^{\lambda_1 t} + (ab)_{32}\, e^{\lambda_2 t} + (ab)_{33}\, e^{\lambda_3 t} = b_{31}\, \lambda_1\, e^{\lambda_1 t} + b_{32}\, \lambda_2\, e^{\lambda_2 t} + b_{33}\, \lambda_3\, e^{\lambda_3 t} \tag{14}$$

From Equation 12 we deduce

$$(ab)_{11} = b_{11}\, \lambda_1$$

and from Equation 13

$$(ab)_{21} = b_{21}\, \lambda_1$$

and from Equation 14

$$(ab)_{31} = b_{31}\, \lambda_1$$

which, written out in full, give

$$\begin{aligned} a_{11}\, b_{11} + a_{12}\, b_{21} + a_{13}\, b_{31} &= b_{11}\, \lambda_1 \\ a_{21}\, b_{11} + a_{22}\, b_{21} + a_{23}\, b_{31} &= b_{21}\, \lambda_1 \\ a_{31}\, b_{11} + a_{32}\, b_{21} + a_{33}\, b_{31} &= b_{31}\, \lambda_1 \end{aligned}$$

or

$$\begin{bmatrix} (a_{11}-\lambda_1) & a_{12} & a_{13} \\ a_{21} & (a_{22}-\lambda_1) & a_{23} \\ a_{31} & a_{32} & (a_{33}-\lambda_1) \end{bmatrix} \begin{Bmatrix} b_{11} \\ b_{21} \\ b_{31} \end{Bmatrix} = 0$$

or

$$(A-\lambda_1 I)b_{i1} = 0 \tag{15}$$

where I is the identity matrix. Similarly, by equating all terms in $e^{\lambda_2 t}$ we obtain

$$(\mathbf{A}-\lambda_2 I)b_{i2} = 0 \tag{16}$$

and equating all terms in $e^{\lambda_3 t}$

$$(\mathbf{A}-\lambda_3 I)b_{i3} = 0 \tag{17}$$

Thus the λ_i are the n eigenvalues of **A**, and the vectors

$$\begin{Bmatrix} b_{11} \\ b_{21} \\ b_{31} \end{Bmatrix}, \begin{Bmatrix} b_{12} \\ b_{22} \\ b_{32} \end{Bmatrix}, \begin{Bmatrix} b_{13} \\ b_{23} \\ b_{33} \end{Bmatrix}$$

are the eigenvectors of **A**.

For each eigenvalue λ_i, the corresponding eigenvector is determined except for an arbitrary multiplier. Thus, supposing that corresponding to each λ_j we obtained the eigenvectors $E_{i,j}$:

Eigenvalues: $\lambda_1 \quad \lambda_2 \quad \lambda_3$

Eigenvectors: $\begin{Bmatrix} E_{11} \\ E_{21} \\ E_{31} \end{Bmatrix} \begin{Bmatrix} E_{12} \\ E_{22} \\ E_{32} \end{Bmatrix} \begin{Bmatrix} E_{13} \\ E_{23} \\ E_{33} \end{Bmatrix}$

then the b_{ij} must obey

$$b_{11} = k_1 E_{11}, \; b_{12}=k_2 E_{12}, \; b_{13}=k_3 E_{13}$$
$$b_{21} = k_1 E_{21}, \; b_{22}=k_2 E_{22}, \; b_{33}=k_3 E_{23} \qquad (18)$$
$$b_{31} = k_1 E_{31}, \; b_{32}=k_2 E_{32}, \; b_{33}=k_3 E_{33}$$

Combining Equations 8 and 18,

$$k_1E_{11} + k_2E_{12} + k_3E_{13} = u_{01} - b_{\infty 1}$$
$$k_1E_{21} + k_2E_{22} + k_3E_{23} = u_{02} - b_{\infty 2}$$
$$k_1E_{31} + k_2E_{32} + k_3E_{33} = u_{03} - b_{\infty 3}$$

or

$$Ek = u_o - b_\infty \qquad (19)$$

and

$$k = E^{-1} (u_o - b_\infty) \qquad (20)$$

where E^{-1} is the inverse of E.

With the determination of the multipliers k, the equation

$$u = b_\infty + Be^{\lambda t}$$

is completely determined, and the function u can be determined for each of the grid points at any time.

EXAMPLE

As an example of the method, the following three-point problem will be solved: Given the differential equation

$$\delta u/\delta t = \alpha\delta^2 u/\delta x^2 + \beta\delta^2 u/\delta y^2 \tag{21}$$

find expressions for u(t) at the three points inside the domain shown in Figure 2. The numbers shown in the figure on the boundary points indicate constant values there, and the numbers in brackets at the internal nodes indicate the initial condition.

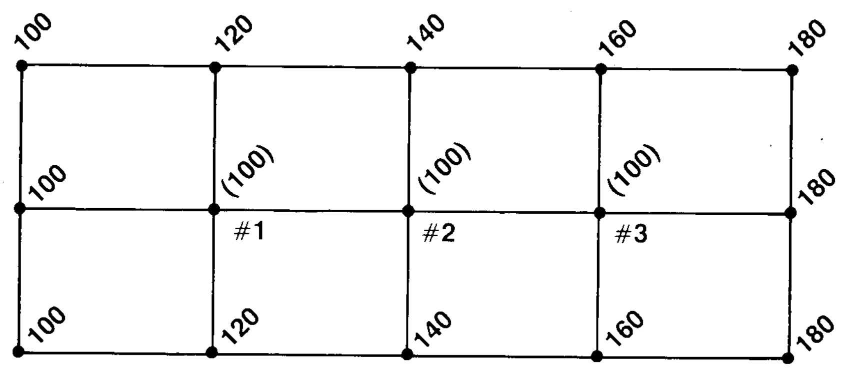

Figure 2. Configuration, initial values, and boundary values of the sample problem.

The first step in the hybrid method is to replace the right-hand side of (21) by a finite approximation, for which we choose

$$\begin{aligned} du/dt = {} & (\alpha/\Delta x^2)\ (u_{i+1,j} - 2u_{i,j}+u_{i-1,j}) \\ & + (\beta/\Delta y^2)\ (u_{i,j+1} - 2u_{i,j} + u_{i,j-1}) \end{aligned} \tag{22}$$

If we choose δx and δy such that

$$\alpha/\Delta x^2 = \beta/\Delta y^2 = p$$

Equation 22 becomes

$$du/dt = p(u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{i,j}) \qquad (23)$$

Writing Equation 23 for each of the interior nodes No. 1, No. 2, and No. 3, and replacing values of u on the boundaries by their constant values, we have

$$du_1/dt = p(340 - 4u_1 + u_2)$$
$$du_2/dt = p(280 + u_1 - 4u_2 + u_3)$$
$$du_3/dt = p(500 + u_2 - 4u_3)$$

or

$$du/dt = p \begin{Bmatrix} 340 \\ 280 \\ 500 \end{Bmatrix} + p \begin{bmatrix} -4 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & -4 \end{bmatrix} \begin{Bmatrix} u_1 \\ u_2 \\ u_3 \end{Bmatrix}$$

Thus

$$\mathbf{A} = p \begin{bmatrix} -4 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & -4 \end{bmatrix}$$

and

$$c = p \begin{Bmatrix} 340 \\ 280 \\ 500 \end{Bmatrix}$$

The inverse of **A** is found to be

$$\mathbf{A}^{-1} = -\frac{1}{56p} \begin{bmatrix} 15 & 4 & 1 \\ 4 & 16 & 4 \\ 1 & 4 & 15 \end{bmatrix}$$

and, from Equation 7,

$$b_{\infty 1} = 120, \; b_{\infty 2} = 140, \text{ and } b_{\infty 3} = 160$$

which are the expected values (Fig. 2) at $t = \to\infty$

The next step is to find λ, the three eigenvalues of **A**; that is, to determine those values of λ for which the determinant

$$\begin{vmatrix} (\lambda+4p) & -p & 0 \\ -p & (\lambda+4p) & -p \\ 0 & -p & (\lambda+4p) \end{vmatrix} = 0$$

They are

$$\lambda_1 = -4p \quad , \quad \lambda_2 = -4p + p\sqrt{2} \quad , \quad \lambda_3 = -4p - p\sqrt{2}$$

Next, find the eigenvectors by substituting λ_1, λ_2, and λ_3 in Equations 15, 16, and 17, respectively. For λ_1 and Equation 15, for example, this gives

$$\begin{bmatrix} 0 & -p & 0 \\ -p & 0 & -p \\ 0 & -p & 0 \end{bmatrix} \begin{Bmatrix} E_{11} \\ E_{21} \\ E_{31} \end{Bmatrix} = 0$$

for which

$$E_{11} = 1, E_{21} = 0, E_{31} = -1$$

is a solution, and thus the eigenvector for $\lambda_1 = -4p$. Similarly the eigenvectors corresponding to λ_2 and λ_3 are determined, and the complete matrix E is

$$E = \begin{bmatrix} 1 & 1 & 1 \\ 0 & \sqrt{2} & -\sqrt{2} \\ -1 & 1 & 1 \end{bmatrix}$$

In the last step, the multipliers k_i are determined from

$$Ek = u_0 - b_\infty$$

or

$$\begin{bmatrix} 1 & 1 & 1 \\ 0 & \sqrt{2} & -\sqrt{2} \\ -1 & 1 & 1 \end{bmatrix} \begin{Bmatrix} k_1 \\ k_2 \\ k_3 \end{Bmatrix} = \begin{Bmatrix} 100-120 \\ 100-140 \\ 100-160 \end{Bmatrix} = \begin{Bmatrix} -20 \\ -40 \\ -60 \end{Bmatrix}$$

from which

$$k_1 = 20$$
$$k_2 = -20 - 20/\sqrt{2}$$
$$k_3 = -20 + 20/\sqrt{2}$$

Thus

$$B = \begin{bmatrix} 20 & (-20-20/\sqrt{2}) & (-20+20/\sqrt{2}) \\ 0 & (-20-20\sqrt{2}) & (-20+20\sqrt{2}) \\ -20 & (-20-20/\sqrt{2}) & (-20+20/\sqrt{2}) \end{bmatrix}$$

and

$$u_1 = 120 + 20e^{-4pt} - 20(1+1/\sqrt{2})e^{-pt(4-\sqrt{2})} - 20(1-1/\sqrt{2})e^{-pt(4+\sqrt{2})}$$
$$u_2 = 140 \qquad - 20(1+\sqrt{2})e^{-pt(4-\sqrt{2})} - 20(1-\sqrt{2})e^{-pt(4+\sqrt{2})}$$
$$u_3 = 160 - 20e^{-4pt} - 20(1+1/\sqrt{2})e^{-pt(4-\sqrt{2})} - 20(1-1/\sqrt{2})e^{-pt(4+\sqrt{2})}$$

Table 1 shows the hybrid solution in comparison with solutions obtained by the Crank-Nicholson method and the forward finite difference method for p = .2.

Table 1. Comparison of Solutions by Three Different Methods

Time	Node	Forward finite difference	Crank-Nicholson	Hybrid method $u = b_\infty + Be^{\lambda t}$
	1	108	106.72	106.65
1	2	116	114.02	114.02
	3	140	129.57	128.67
	1	112.8	111.31	111.23
2	2	128.8	123.98	123.79
	3	151.2	143.96	143.15
	1	116.32	114.44	114.35
3	2	134.56	130.35	130.09
	3	156.00	151.29	150.72
	1	118.18	116.52	116.42
4	2	137.38	134.25	134.01
	3	158.11	155.17	154.79
	1	119.11	117.85	117.77
5	2	138.73	136.59	136.40
	3	159.10	157.28	157.04
	1	119.79	119.21	119.16
7	2	139.70	138.82	138.71
	3	159.79	159.11	159.01

CONCLUSION

Solution by the hybrid method is carried out in six steps:

1. Define matrix **A** and vector c from the problem definition.
2. Compute the inverse of **A** and the steady state vector b using Equation 7.
3. Compute the eigenvalues and eigenvectors of **A**, the eigenvectors forming matrix E, columnwise.
4. Compute the multipliers k_i from

   $$Ek = u_0 - b_\infty$$

   or

   $$k = E^{-1}\ (u_o - b_\infty)$$

5. Compute the matrix B by multiplying the jth column of E by k_j:

   $$b_{ij} = k_j E_{ij}$$

6. Calculate the value of the function u at any node for any time from

   $$u = b_\infty + Be^{\lambda t}$$

Suitable routines for the calculation of eigenvalues and eigenvectors can be found, for example, in Wilkinson (1965) or Smith *et al.* (1974).

The hybrid method is still in the experimental stage; it has performed adequately on a 20-point problem, but the behaviour in larger problems is as yet unknown.

No data have been compiled so far on the speed of the hybrid solution in comparison with standard methods; efficiency of the method will depend largely on the availability of fast numerical routines to find eigenvalues of large, but sparse, matrices.

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