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MIXED EXPLICIT-IMPLICIT ITERATIVE FINITE ELEMENT SCHEME FOR DIFFUSION-TYPE PROBLEMS: II. SOLUTION STRATEGY and EXAMPLES

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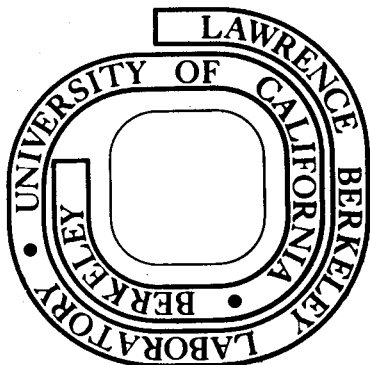
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MIXED EXPLICIT-IMPLICIT ITERATIVE FINITE ELEMENT SCHEME
FOR DIFFUSION-TYPE PROBLEMS:
II. SOLUTION STRATEGY AND EXAMPLES

by

T. N. Narasimhan,¹ S. P. Neuman,^{1,2}
and A. L. Edwards³

Summary

In Part I¹ of this paper we have established local stability and convergence criteria for the mixed explicit-implicit finite element scheme and have shown that the proposed iterative method converges under certain conditions. Part II describes various practical aspects of the solution strategy such as convergence criteria for terminating the iterations, automatic control of time step size, reclassification of nodes from explicit to implicit during execution, estimation of time derivatives, and automatic adjustment of the implicit weight factor. Several examples are included to demonstrate certain aspects of the theory and illustrate the capabilities of the new approach.

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Introduction

In Part I of this paper¹ we introduced the following explicit-implicit finite element expression for diffusion-type problems (see (27) in Part I):

$$\Delta h_n = \sum_{m \neq n} \lambda_{nm} \left[\underbrace{(h_n^k - h_m^k)}_{\text{Explicit part}} + \theta \underbrace{(\Delta h_n - \Delta h_m)}_{\text{Implicit part}} \right] + Q_n \Delta t / D_{nn}^*$$

$$n = 1, 2, \dots, N \quad (1)$$

where h_n^k is the dependent variable (hydraulic head in the case of groundwater flow) at node n and time step k , $\Delta h_n = h_n^{k+1} - h_n^k$, λ_{nm} represents the off-diagonal terms of a matrix $[\underline{\lambda}]$ defined in equation (7) of Part I, θ is a weighting factor defined within the range $0 \leq \theta \leq 1$, Q_n is a sink or source term, and N is the total number of nodes. Application of the point accelerated iterative method of Evans et al.² to (1) leads to the algorithm (see (28) in Part I¹)

$$\Delta h_n^{j+1} = \frac{\sum_{m \neq n} \lambda_{nm} (h_n^k - h_m^k) - \theta \sum_{m \neq n} \lambda_{nm} (g \Delta h_n^j + \Delta h_m^j) + Q_n \Delta t / D_{nn}^*}{1 - \theta (1 + g) \sum_{m \neq n} \lambda_{nm}} \quad (2)$$

where j is the number of iterations and g is an acceleration factor the optimum value of which is approximately 0.2.

In Part I we have established local stability and convergence criteria for the finite element scheme in (1) and have shown that the iterative method in (2) converges under certain conditions. The purpose of Part II is to describe various practical aspects of the solution strategy including the iteration technique and associated convergence criteria, automatic control of time step size, reclassification of nodes from explicit to implicit during execution, estimation of time derivatives, and automatic

adjustment of the implicit weight factor, θ . In addition, several examples are included to demonstrate certain aspects of the theory and illustrate the capabilities of the new approach.

Mixed Explicit-Implicit Solution Strategy

The local nature of the stability criteria for (1), together with the use of a point iterative technique, suggest the interesting possibility of solving the finite element equations explicitly at some nodes and implicitly at other nodes during a single time step. If Δt satisfies the stability condition (18) in Part I for some node n , then equation (1) can be solved explicitly for Δh_n at that node. At nodes which do not satisfy the stability criterion, Δh_n is determined iteratively by using the algorithm in (2). A final correction is then made to the Δh_n values calculated explicitly, when required to conserve mass. We refer to this approach as a mixed explicit-implicit solution strategy.

The mixed strategy is very useful in dealing with meshes characterized by a significant spatial variability of element sizes and material properties. For example, if the region of interest consists of two materials having different conductivities and capacities, it may sometimes be possible to solve explicitly in one material and implicitly in the other. The mixed approach is also useful when there is a sudden change in boundary conditions. In this case it is often desirable to use small Δt values for a short period of time until the system reaches a certain level of equilibrium, otherwise there may be a loss of accuracy. The attractive possibility of using an explicit solution procedure during this period may lead to significant savings in computer time.

The idea of combining explicit and implicit calculations in a single time step was previously used in conjunction with an integrated finite difference scheme by Edwards.³ The procedure has been incorporated by

Edwards into a powerful computer program, called TRUMP, which can handle multidimensional steady state and transient temperature distributions in complex, non-uniform, and isotropic systems, taking into account conduction, convection, and radiation. The program has also been applied by Edwards⁴ to darcian fluid flow in porous media. The conduction aspects of TRUMP are based on a set of algebraic equations which have the same general form as (1). This made it possible for us to develop a computer program which combines the advantages of the finite element method (such as the ability to treat anisotropic regions with complex geometry) with the remarkable logic and facilities of TRUMP. The new program is called FLUMP, as a mnemonic for Finite eLement and trUMP.

In addition to the mixed explicit-implicit solution strategy, the user of FLUMP has the option of using a fully explicit forward difference scheme ($\theta = 0$), a time-centered Crank-Nicholson scheme ($\theta = 0.5$), or a fully implicit backward difference scheme ($\theta = 1.0$), throughout any part of the solution process. However, in practice these options are seldom used because FLUMP has the facility to adjust the weight factor θ automatically during execution in a manner that ensures a high level of accuracy at each time step. This, as well as other special features of FLUMP, are described briefly below.

Iteration Technique

The iteration algorithm is based on equation (2). During a given time step, Δt , the algorithm is applied only to a selected number of nodes (called implicit nodes) which cannot be treated explicitly without endangering stability. In the computer program the iterations are performed in terms of residuals, defined as $\epsilon_n^{j+1} = \Delta h_n^{j+1} - \Delta h_n^j$. Substituting these residuals

into (2) and rearranging leads to the computational algorithm

$$\epsilon_n^{j+1} = \frac{-\theta \sum_{m \neq n} \lambda_{nm} (g \epsilon_n^j + \epsilon_m^j)}{1 - \theta (1 + g) \sum_{m \neq n} \lambda_{nm}} \quad (3)$$

For the first iteration ($j = 0$), the following initial guesses are used,

$$\begin{aligned} \Delta h_n^0 &= \dot{h}_n \Delta t \\ \Delta h_m^0 &= \dot{h}_m \Delta t \end{aligned} \quad (4)$$

where \dot{h}_n and \dot{h}_m are estimated time derivatives (a method for obtaining these derivatives is described later in the text). The values of Δh_n^1 are then calculated using (2), and the first set of residuals is determined according to the formula

$$\epsilon_n^1 = \Delta h_n^1 - \dot{h}_n \Delta t \quad (5)$$

The next set of residuals, ϵ_n^2 , is calculated with (3), and Δh_n^2 is found from the relation

$$\Delta h_n^{j+1} = \Delta h_n^j + \epsilon_n^{j+1} \quad (6)$$

This procedure is continued with the aid of (3) and (6) until convergence is achieved or, until 80 iterations have been completed. In the latter case, the calculations are repeated with half the original value of Δt . This may continue until Δt reaches a minimum specified value, in which case execution terminates with a diagnostic message.

Two convergence criteria must be satisfied simultaneously before terminating the iterations. The first criterion is

$$\max_n |\epsilon_n^j| \leq 10^{-4} \Delta h_{des} \quad (7)$$

where Δh_{des} is the desired maximum change in h at any node during a time step (as will be seen later, Δt is adjusted during execution to maintain the maximum change in h near the value of Δh_{des} , and less than $2\Delta h_{des}$). The second criterion is based on the net correction to fluid content and the net fluid capacity of all implicit nodes, defined as

$$\Delta H_{net}^j = \left| \sum_n D_{nn}^* \epsilon_n^j \right| \quad (8)$$

$$D_{net}^* = \sum_n D_{nn}^* \quad (9)$$

where the summation is taken over all implicit nodes. The iterative procedure is stopped when (7) is satisfied together with (10) below,

$$\Delta H_{net}^j < 10^{-5} D_{net}^* \Delta h_{des} \quad (10)$$

i.e., the net error in fluid content is less than 10^{-5} of the amount of fluid required to change h at all implicit nodes by the amount Δh_{des} . Experiments by Edwards³ on a large number of sample problems using TRUMP indicate that the net cumulative error in the average value of h tends to be no more than $0.01 \Delta h_{des}$ after several hundred time steps; the cumulative error at individual nodes does not usually exceed $0.1 \Delta h_{des}$, and is much less if some values of h are fixed at the boundary of the system.

After having completed the iterative procedure for all implicit nodes, one must now correct the values of h at all explicit nodes connected to implicit nodes, according to (see equation (1))

$$\Delta h_n^{\text{explicit corrected}} = \Delta h_n^{\text{explicit}} + \theta \sum_{m \neq n} \lambda_{nm} (\Delta h_n - \Delta h_m) \quad (11)$$

where the summation is taken only over implicit nodes. This correction is necessary for a correct material balance. Since in FLUMP internal fluxes between adjacent subregions are calculated simultaneously with the h values as explained in Part I,¹ these fluxes must also be corrected in a similar manner.

Control of Time Step Size

The size of Δt in FLUMP is controlled by several factors such as the lower and upper limits specified by the user (Δt_{low} and Δt_{high} , respectively), the desired maximum change in h at any node during a time step (Δh_{des}), the smallest time step allowed at any explicit node by the stability criterion (18) in Part I¹ (Δt_{stab}), the average number of iterations required for convergence, and the desired interval between printed outputs.

The first time step is always 10^{-12} and is used primarily for checking the input data, establishing time derivatives, and determining Δt_{stab} (the latter is recalculated whenever the conductance or capacity matrices change). The maximum allowed time step, Δt_{max} , is then set equal to $2/3$ of Δt_{stab} or Δt_{high} , whichever is smallest (the use of $2/3$ of Δt_{stab} instead of Δt_{stab} greatly increases the accuracy in coarse meshes). The minimum allowed time step, Δt_{min} , is set equal to Δt_{low} or 10^{-10} , whichever is greater. If Δt_{low} is equal to or greater than Δt_{max} , the value of Δt_{min} is reduced to slightly less than Δt_{max} so as to prevent the input value from causing instabilities. The default value for Δt_{low} is taken to be $\Delta t_{\text{max}}/100$.

During the subsequent calculations the size of Δt is gradually adjusted to obtain a maximum change in h close to Δh_{des} and not exceeding $2\Delta h_{\text{des}}$, to maintain the maximum change in any tabulated material property in nonlinear problems near 1% or less and not exceeding 2%, and to prevent the number of

iterations from averaging more than 40, the maximum allowed being 80. The technique for doing this has been designed by Edwards³ so as to cause a rapid decrease in Δt when the above limits are exceeded, with a more gradual increase in Δt when changes are relatively slow. For this purpose, let δ be either the largest percentage change that took place during the recent time step in any tabulated property, or 1/40 of the number of iterations required for convergence, whichever is larger. We then calculate the ratio

$$R = \Delta h_{des} / \max \left(\max_n |\Delta h_n|, \delta \Delta h_{des} \right) \quad (12)$$

and if $R \leq 0.5$ and $\Delta t \geq 1.01 \Delta t_{min}$, the entire computation for the recent time step is repeated with a modified value of Δt . If all the nodes in the mesh are set to be implicit, R is reduced by a factor of 100 for the first time step to start the calculation out smoothly. If $R \leq 1.0$, the new time step is calculated according to

$$\Delta t_{new} = R^2 \Delta t_{old} \quad (13)$$

whereas if $R > 1$, the formula is

$$\Delta t_{new} = 0.5 (1 + R) \Delta t_{old} \quad (14)$$

In both cases the adjustments are subject to the constraints $\Delta t_{min} \leq \Delta t_{new} \leq \Delta t_{max}$ and $0.5 \Delta t_{old} \leq \Delta t_{new} \leq 2.0 \Delta t_{old}$.

An additional adjustment in the size of Δt may be required in order to meet a desired interval between printed outputs. For details of this adjustment procedure the reader is referred to Edwards.³

Reclassification of Nodes

If the recent time step was equal to Δt_{\max} and less than Δt_{high} , the stability limits of all explicit nodes are tested. All explicit nodes with stability limits equal to or less than $1.8 \Delta t_{\max}$ are then reclassified as implicit nodes. Since $\Delta t_{\max} = (2/3) \Delta t_{\text{stab}}$, the reclassification affects all explicit nodes having stability limits from 1.0 to 1.2 times Δt_{stab} . This range was chosen empirically by Edwards³ in an effort to minimize the required computation time for a large group of test problems using TRUMP.

The rate at which the nodes are reclassified from explicit to implicit depends on the input parameter Δh_{des} ; the larger is this parameter, the faster is the increase in the size of Δt , and therefore the stability limits of most nodes are reached earlier.

Estimation of Time Derivatives

The initial guess of h for the iterative procedure requires a preliminary estimate of the time derivatives, \dot{h} , as has been indicated in (4). In nonlinear problems, the time derivatives are also used to estimate the average values of h to be used in evaluating h -dependent parameters. Rather than saving h_n values from several preceding time steps, which could be used to calculate more accurate time derivatives, a simpler method is used which requires less memory space and machine time, and is sufficiently accurate for most problems.

In FLUMP, the time derivatives for any time step $\Delta t_{k+1} = t_{k+1} - t_k$ are estimated from the maximum rates of change in h occurring during the two preceding time steps, $\Delta t_k = t_k - t_{k-1}$ and $\Delta t_{k-1} = t_{k-1} - t_{k-2}$. For this purpose let us define the two ratios

$$R_k = \max_n \left| \frac{h_n^k - h_n^{k-1}}{\Delta t_k} \right| \bigg/ \max_n \left| \frac{h_n^{k-1} - h_n^{k-2}}{\Delta t_{k-1}} \right| \quad (15)$$

$$R_t = \frac{\Delta t_k + \Delta t_{k+1}}{\Delta t_{k-1} + \Delta t_k} \quad (16)$$

where $0.5 \leq R_t \leq 2.0$ because, as will be recalled, Δt is not allowed to vary from one time step to another by more than a factor of 2. If $R_k < 1.0$, the maximum rate of change in h is decreasing with time, and the estimate is based on the assumption that all h values are approaching equilibrium exponentially according to the formula $h(t) = h(o)e^{-\alpha t}$. Since $e^{-\alpha} = [\dot{h}(t)/\dot{h}(o)]^{1/t}$, it follows that

$$R_{k+1}^{est} = R_k^{R_t} \quad (17)$$

where $R_{k+1}^{est} \leq 1$ is the estimated value of R_{k+1} . If $R_k > 1$, the maximum rate of change in h is increasing, and the estimate is based on the assumption that all h values vary quadratically according to the formula $h(t) = h(o) + \dot{h}(o)t + \alpha t^2$. Since $\dot{h}(t)/\dot{h}(o) - 1 = 2\alpha t/\dot{h}(o)$, it follows that

$$R_{k+1}^{est} = 1 + (1 - R_k^{-1}) R_t \quad (18)$$

where $1 \leq R_{k+1}^{est} \leq 3$ due to the limits imposed on R_t . Equation (18) gives a more conservative estimate of the maximum rate of change in h than (17) does. The estimated time derivative at each node is calculated as the product of the actual derivative during the previous time step and R_{k+1}^{est} ,

$$\dot{h}_n = R_{k+1}^{est} \frac{h_n^k - h_n^{k-1}}{\Delta t_k} \quad (19)$$

Numerical experiments with TRUMP led Edwards³ to conclude that it is advisable to keep $R_{k+1}^{est} = 1.0$ during the first two time steps (a) at the beginning of each problem, (b) after repeating a time step with a modified Δt , and (c) after a node has been reclassified from explicit to implicit. Edwards further concluded that the time derivatives should be set equal to zero or a very small number during the initial time step ($\Delta t = 10^{-12}$) as

well as when they change sign. It was also found that more accurate results can be obtained for implicit nodes having stability limits smaller than Δt_k by estimating their time derivatives during the first two time steps according to

$$\dot{h}_n = (h_n^k - h_n^{k-1})/\Delta t_k \left(1 - \sum_{n \neq m} \lambda_{nm}\right) \quad (20)$$

where the values of λ_{nm} correspond to the time step just completed, Δt_k .

Estimation of Implicit Weight Factor

In most implicit procedures it is customary to employ either a time-centered scheme with $\theta = 0.5$, or a backward difference scheme with $\theta = 1.0$. In FLUMP, θ is allowed to be zero for explicit nodes, or to vary between 0.57 and 1.0 for implicit nodes. Experience indicates that small oscillations caused by rapid changes in boundary conditions or variable parameters tend to persist when θ is close to 0.5. The lower limit of 0.57 was chosen empirically by Edwards³ to eliminate persistent oscillations and to optimize the stability and accuracy of a large number of test problems using TRUMP.

The average value of h at any node during a time step is calculated in the program as $\bar{h}_n = h_n^k + \theta (h_n^{k+1} - h_n^k)$. Let us assume that h approaches equilibrium exponentially. Then for small time steps and for time steps during which the slope of h remains nearly constant, the correct average value is obtained with $\theta = 0.5$. On the other hand, for large time steps near equilibrium, the correct average value is obtained with $\theta = 1.0$. Thus, θ should be in the vicinity of 0.57 during the period when rapid changes in h take place, and should gradually shift toward 1.0 as equilibrium is approached, otherwise there may be a loss of accuracy. One way to accomplish this is by using the empirical formula

$$\theta = \max [0.57, \max (1.0, R_{k+1}^{\text{est}})/(1.0 + R_{k+1}^{\text{est}})] \quad (21)$$

suggested by Edwards³ and this is the approach adopted in FLUMP.

Experiments conducted by Edwards³ on a large number of problems using TRUMP have shown that approach to equilibrium is usually too rapid when a forward difference or time-centered scheme is used, and much more accurate results can be obtained with a variable θ . His experiments also showed that θ should be set equal to 1.0 during the initial time step ($\Delta t = 10^{-12}$) as well as during any time step following a rejected time step. This enables nodes with small stability limits to reach equilibrium with their neighbors when there is a rapid change in a boundary condition or a variable parameter, without overshoot which may lead to damped oscillations.

As mentioned earlier, the computer program also provides an option to fix the value of θ at 0.5, or 1.0 for the entire period of computation, corresponding to explicit forward difference, time-centered, or backward difference schemes, respectively. However, experiments conducted by Edwards³ using TRUMP as well as the examples given in this paper indicate that this tends to reduce accuracy and increase computer time, and is therefore not advisable. The purpose of including these options is to allow the calculational results and machine time to be compared with other methods using a fixed value of θ .

Additional Features of FLUMP

The iterative nature of our solution process makes it ideally suited for the handling of quasilinear diffusion-type problems. Although this feature of the program will not be demonstrated here, we mention in passing that FLUMP can handle problems in which nodal conductivities, capacities, and sources or sinks are tabulated functions either of time or of the dependent variable, h . The boundary conditions can also be controlled in a similar manner by tabulating them as functions of time or h .

The printed output of FLUMP provides information on the nodal values of h , Δh , and estimated values of \dot{h} at discrete time intervals specified by the user. Additional information includes the amount of fluid contained in the exclusive subdomain of each node, change in the amount of fluid in each subdomain during Δt as well as from the start of the problem, total fluid content in the system, flux across the boundary of the system, and the net flux into or out of the exclusive subdomain of each node. This makes it possible to maintain a continuous check on material balance in the subdomain of each node as well as in the system as a whole.

The program also includes a built-in safety feature to warn the user about nodes at which the matrix $[\underline{\lambda}]$ is not diagonally dominant. If the degree of deviation from local diagonal dominance is significant, there is a risk that the solution may be locally unstable (if the node is explicit) and inaccurate, and that convergence will be relatively slow. The problem can always be remedied by locally redesigning the finite element mesh according to the guidelines given in Part I.¹ Since the numbering of nodes and elements is completely arbitrary (as opposed to direct methods such as Gaussian elimination in which numbering has an effect on the band width), local modifications of the mesh can be easily introduced merely by changing a few cards in the data deck.

Examples

The purpose of the following examples is to demonstrate certain aspects of the theory and illustrate some of the capabilities of our new approach.

Example 1: Our first example concerns the solution of a one-dimensional problem with a two-dimensional finite element network. The problem is to solve the partial differential equation

$$\frac{\partial^2 h}{\partial x^2} = \frac{\partial h}{\partial t} \quad ; \quad 0 \leq x \leq 1 \quad ; \quad t \geq 0 \quad (22)$$

subject to the initial and boundary conditions

$$\begin{aligned} h(x, 0) &= 1 \\ h(0, t) &= h(1, t) = 0 \end{aligned} \quad (23)$$

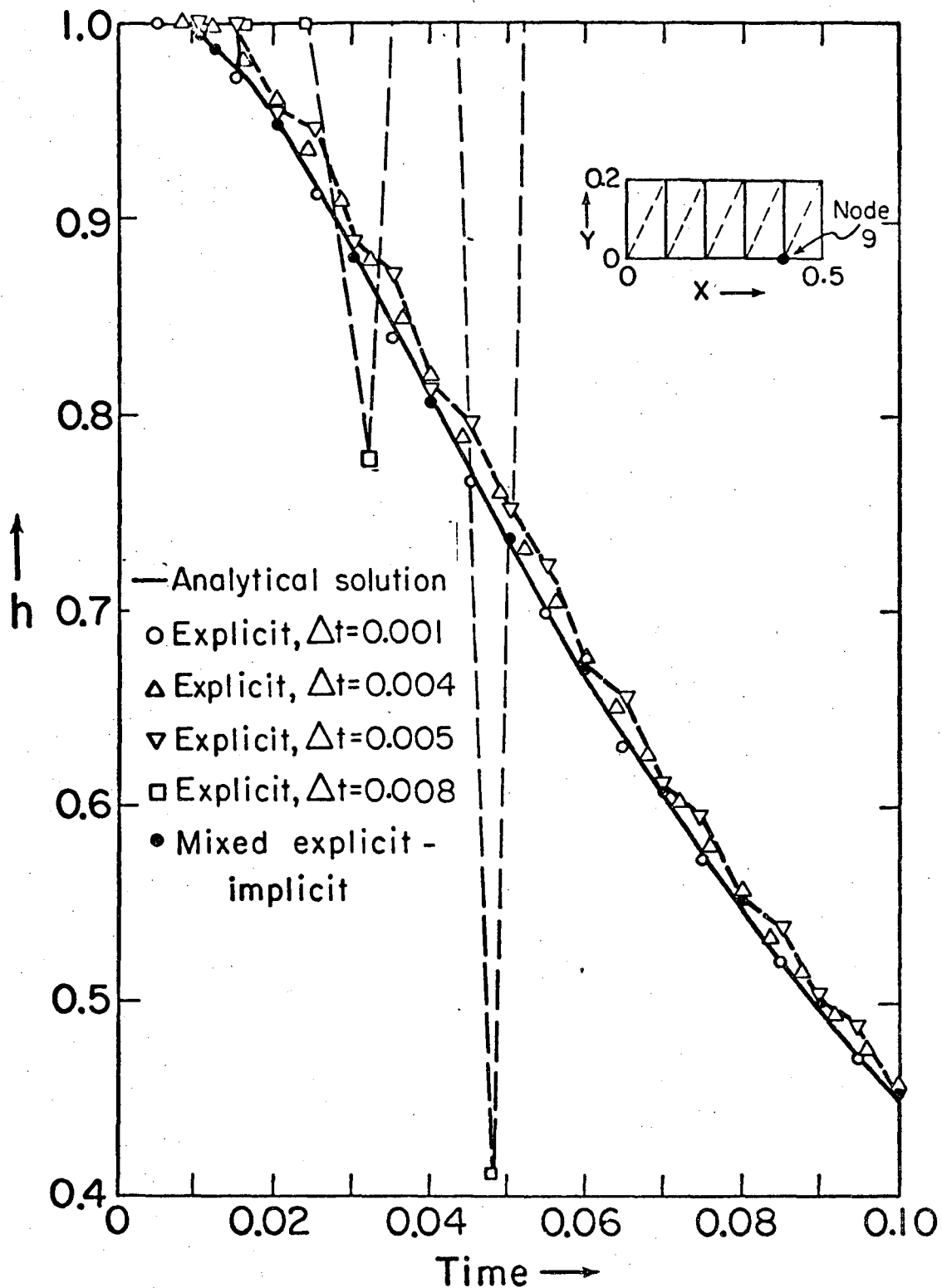
The exact solution is given by O'Brien et al.⁵ as

$$h(x, t) = \frac{4}{\pi} \sum_{n=1,3,5,\dots}^{\infty} n^{-1} e^{-n^2 \pi^2 t} \sin(n \pi x) \quad (24)$$

Physically, this may represent the decline of hydraulic head in a rock core sample having a hydraulic conductivity and compressive capacity of unity.

The two-dimensional finite element network used to solve the problem is shown as an inset in Figure 1 (only one half of the flow field needs to be considered because the solution is symmetric about $x = 0.5$). The thickness of the network in the y direction was arbitrarily set equal to 0.2. The stability limit of all internal nodes in this mesh was calculated by FLUMP to be 0.004; the stability limits of the four nodes lying on the boundary ($x = 0$ and $x = 0.5$) were different due to the asymmetry of the mesh, and these nodes were therefore treated as implicit at all times.

In order to check whether our method of calculating stability limits is correct, we solved the problem using various fixed Δt values while maintaining θ at all internal nodes equal to zero (i.e., treating these nodes explicitly at all times). Figure 1 shows the analytical solution for $x = 0.4$ together with numerical results calculated explicitly at node 9 (see inset) by using fixed Δt values equal to 0.001, 0.004, 0.005, and 0.008. It is seen that the solutions corresponding to $\Delta t \leq 0.004$ (i.e.,



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Figure 1. One-dimensional problem: Examination of stability at node 9.

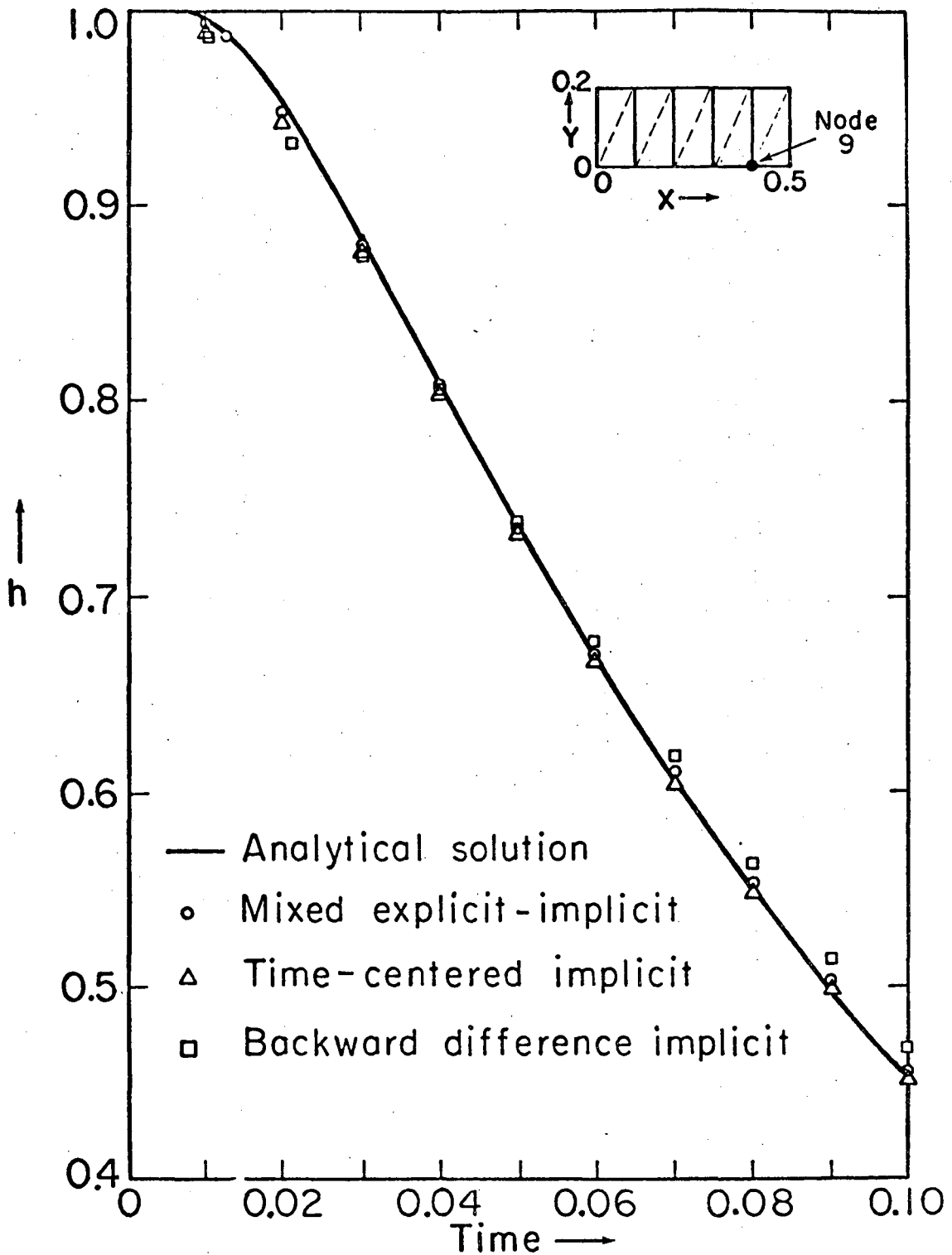
less than or equal to the theoretical stability limit) are stable as we would expect. The solution corresponding to $\Delta t = 0.005$, which slightly exceeds the stability limit, is less accurate and exhibits low-amplitude oscillations. The solution obtained with $\Delta t = 0.008$ is completely unstable.

Figure 1 also shows results obtained with the mixed explicit-implicit approach which uses a variable Δt , with the maximum value of Δt set equal to 0.01. In terms of accuracy, these results are comparable to those obtained explicitly with a much smaller time step, $\Delta t = 0.001$. In terms of execution time, the mixed approach is faster: It required 0.527 seconds on the CDC 7600, whereas the explicit scheme with $\Delta t = 0.001$ required 0.823 seconds to reach the maximum time of $t = 0.1$.

Figure 2 shows a comparison between the mixed explicit-implicit scheme and two implicit schemes, time-centered and backward difference. All three solutions were obtained with a variable Δt , the maximum allowed time step being 0.01. It is seen that the mixed scheme is the most accurate at early time, and is comparable in accuracy to the time-centered scheme at later times; the backward difference scheme gives the least accurate results. The mixed approach is also the most economical one from the standpoint of computer time: It reached $t = 0.1$ in 20 time steps and 118 iterations, requiring 0.527 seconds for execution on the CDC 7600. The time-centered scheme reached $t = 0.1$ in 26 time steps and 133 iterations, requiring 0.571 seconds for execution, whereas the backward difference scheme reached $t = 0.1$ in 25 time steps and 191 iterations, requiring 0.587 seconds for execution.

Example 2: In the second example we want to solve the partial differential equation

$$K_x \frac{\partial^2 h}{\partial x^2} + K_y \frac{\partial^2 h}{\partial y^2} = \frac{\partial h}{\partial t}; \quad 0 \leq x, y \leq 1; \quad t \geq 0 \quad (25)$$



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Figure 2. One-dimensional problem: Comparison of results at node 9 obtained by backward difference, time-centered, and mixed explicit-implicit schemes.

subject to the initial and boundary conditions

$$\begin{aligned}
 h(x, y, 0) &= 0 \\
 h(1, y, t) &= h(x, 0, t) = 1 \\
 \frac{\partial h}{\partial x}(0, y, t) &= \frac{\partial h}{\partial y}(x, 1, t) = 0
 \end{aligned} \tag{26}$$

The exact solution can be obtained from Olson and Schultz⁶ and is given by Bruch and Zyvoloski⁷ as

$$\begin{aligned}
 h(x, y, t) &= 1 + \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} C_{nm} \cos [0.5 (2n-1) \pi x] \cos [0.5 (2m-1) \pi y] \\
 &\quad \cdot \exp \{-0.25 \pi^2 t [K_x (2n-1)^2 + K_y (2m-1)^2]\}
 \end{aligned} \tag{27}$$

where

$$C_{nm} = - \frac{16 (-1)^{n+1} (-1)^{m+1}}{\pi^2 (2n-1) (2m-1)}$$

Physically, this may represent the rise of hydraulic head in an infinite anisotropic porous medium of square cross section with its principal conductivities oriented parallel to the sides of the square and having a compressive capacity of unity. We will consider two cases with different ratios between the conductivities K_x and K_y .

Case 1: The first case is that of an isotropic medium with $K_x = K_y = 1$. The finite element network used to solve the problem is shown as an inset in Figure 3. The stability limit of all but one of the nodes at which h is unknown was calculated by FLUMP to be 0.0025; only at one corner node was the limit lower and this node was therefore set to be implicit at all times.

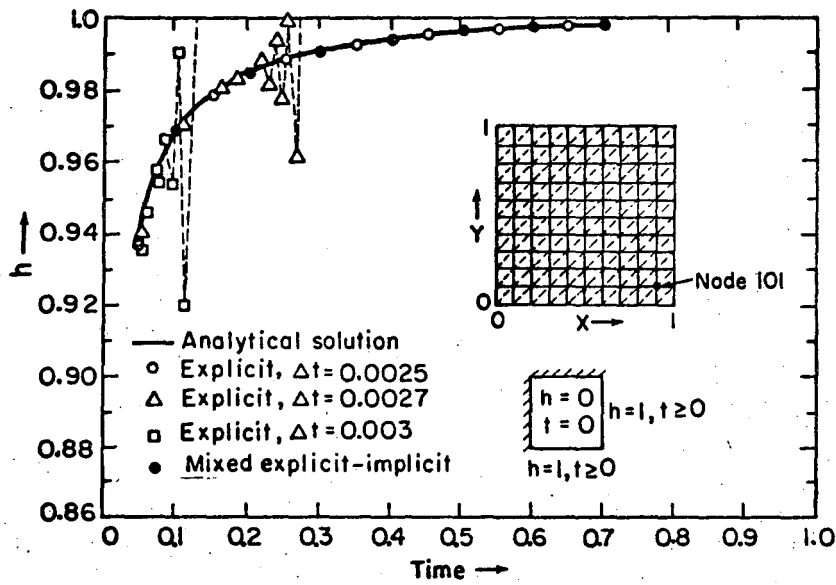
To check the validity of this theoretical stability limit, we solved the problem using various fixed Δt values by treating all but one corner

node explicitly at all times. Figure 3 shows the analytical solution for $x = 0.9$ and $y = 0.1$ together with numerical results calculated explicitly at node 101 (see inset) by using fixed Δt values equal to 0.0025, 0.0027, and 0.003. It is seen that the solution corresponding to $\Delta t = 0.0025$ (i.e., equal to the theoretical stability limit) is stable as we would expect. The solution corresponding to $\Delta t = 0.0027$, which slightly exceeds the stability limit, becomes unstable after $t = 0.2$. The solution obtained with $\Delta t = 0.003$ becomes unstable at an earlier time, $t = 0.1$.

Figure 4 has been included to illustrate the nature of the spatial instabilities that may develop when an explicit scheme is used with too large a time step. The results correspond to two cross sections, A-A', at $t = 0.05$.

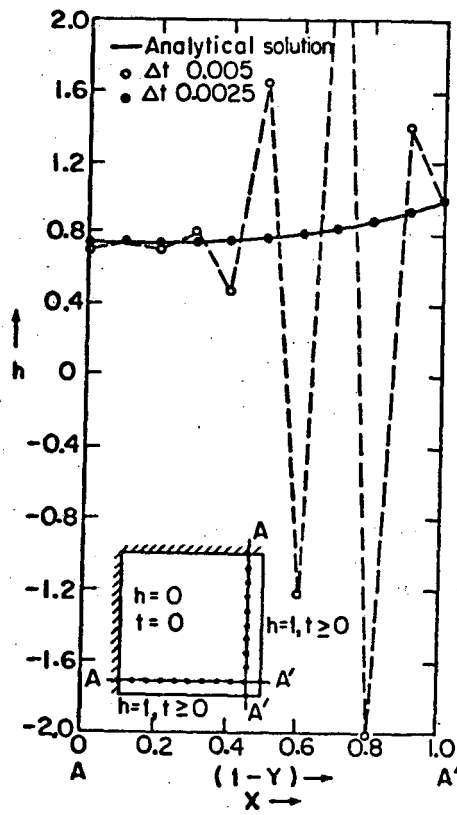
Figure 3 also shows results obtained with the mixed explicit-implicit approach which uses a variable Δt , with the maximum value of Δt set equal to 0.05. In terms of accuracy, these results are comparable to those obtained explicitly with a much smaller time step, $\Delta t = 0.0025$. In terms of execution time, the mixed approach is faster: It required 2.351 seconds on the CDC 7600 to reach $t = 1.0$, whereas the explicit scheme with $\Delta t = 0.0025$ required 4.653 seconds to reach the same time.

Figure 5 shows a comparison between the mixed explicit-implicit scheme and two implicit schemes, time-centered and backward difference, at node 61 (see inset). All three solutions were obtained with a variable Δt , the maximum allowed time step being 0.05. It is seen that the mixed and time-centered schemes are extremely accurate, whereas the backward difference scheme is slightly in error. The mixed approach is the fastest: It reached $t = 1.0$ in 36 time steps and 509 iterations, requiring 2.351 seconds for execution on the CDC 7600. The time-centered scheme reached



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Figure 3. Two-dimensional isotropic problem: Examination of stability at node 101.



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Figure 4. Two-dimensional isotropic problem: Examination of spatial instability.

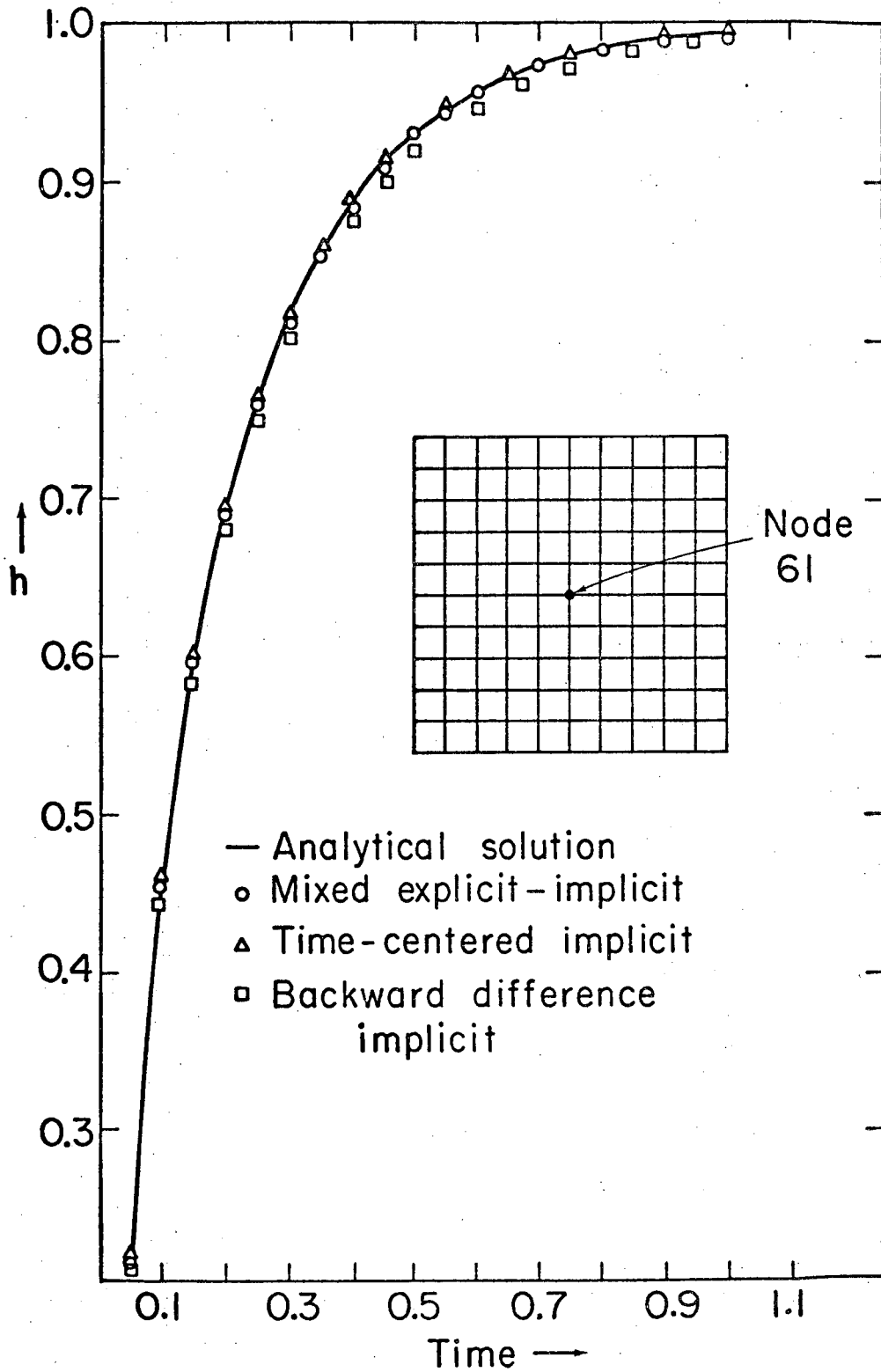


Figure 5. Two-dimensional isotropic problem: Comparison of results at node 61 obtained by backward difference, time-centered, and mixed explicit-implicit schemes.

$t = 1.0$ in 43 time steps and 507 iterations, requiring 2.493 seconds for execution, whereas the backward difference scheme used 50 time steps and 904 iterations, requiring 3.617 seconds for execution.

Bruch and Zyvoloski⁷ published results obtained by them at $t = 0.75$ with a constant time step, $\Delta t = 0.05$, by using rectangular prism elements in the space-time domain. Table I compares our results with theirs and shows that the use of a variable Δt leads to more accurate results. Bruch and Zyvoloski⁷ also reported that by using a constant time step, $\Delta t = 0.05$, they obtained physically unreasonable values of h (greater than 1) near the constant h boundaries at the end of the first time step, resulting in damped oscillations for several subsequent time steps. A similar phenomenon was observed by Carnahan et al.⁸ in solving this problem with the alternating direction implicit procedure. Such difficulties are avoided in FLUMP owing to the manner in which Δt is controlled by the program.

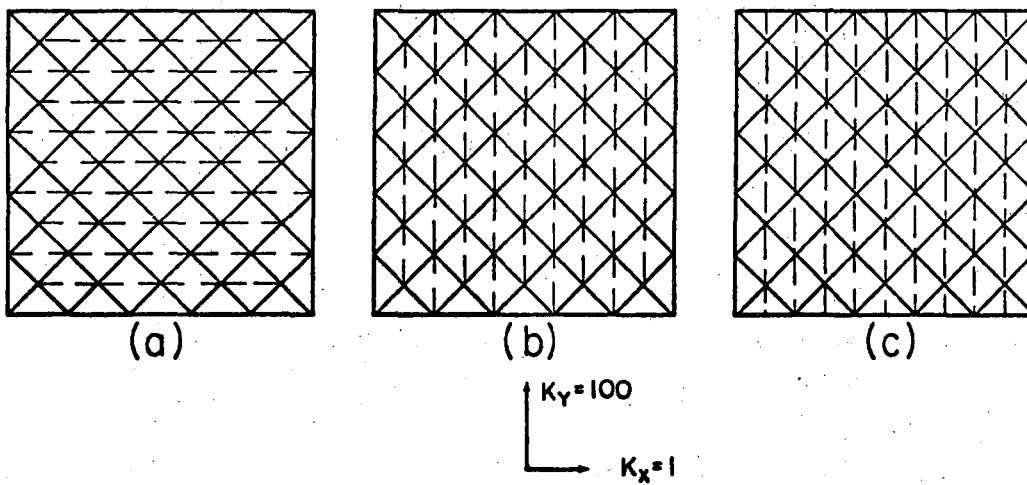
Case 2: The second case is that of an anisotropic medium with $K_x = 1$ and $K_y = 100$. The problem was first solved by adopting the same finite element network as that used for the isotropic problem (see inset in Figure 3). Since contracting the network parallel to the y axis or expanding it parallel to the x axis does not cause any of the angles to become obtuse, the matrix $[\underline{\lambda}]$ is diagonally dominant, and we therefore expect the solution process to converge.

Tables II and III compare results obtained with the mixed, time-centered, and backward difference schemes at $t = 0.002$ and $t = 0.01$, respectively. All three sets of results were obtained with a variable Δt , the maximum allowed time step being $\Delta t = 0.002$ for $0 \leq t \leq 0.016$ and $\Delta t = 0.01$ for $0.016 < t \leq 0.04$. It is seen that the mixed scheme is only

slightly less accurate than the time-centered scheme, and both are considerably more accurate than backward differences. The mixed approach is again the fastest: It reached $t = 0.04$ in 36 time steps and 547 iterations, requiring 2.459 seconds for execution on the CDC 7600. The time-centered scheme used 43 time steps and 581 iterations requiring 2.596 seconds for execution, whereas the backward difference scheme used 50 time steps and 926 iterations which took 3.422 seconds to execute.

In order to check the effect of diagonal dominance on the quality of the results, we solved the same problem with three different meshes having nearly the same number of elements and nodes, as illustrated in Figure 6. If we contract the mesh in Figure 6A by a factor of ten parallel to the y coordinate so as to see what shape it takes in the equivalent isotropic domain, we find that most of the triangles include a large obtuse angle. As a result of this, the matrix $[\underline{\lambda}]$ is nowhere diagonally dominant (a check on diagonal dominance is performed by FLUMP at each node). The mesh in Figure 6B leads to a matrix which is diagonally dominant everywhere except at nodes lying in the immediate neighborhood of the bottom ($y = 0$) and top ($y = 1$) boundaries, whereas the matrix resulting from the mesh in Figure 6C is diagonally dominant at all nodes.

The results obtained from all three meshes at $t = 0.002$ and $t = 0.01$ are compared with the analytical solution in Tables IV and V, respectively. The number of time steps, number of iterations, and execution time required to reach $t = 0.04$ are compared in Table VI. It is evident from these tables that as the relative number of nodes at which $[\underline{\lambda}]$ is diagonally dominant increases, the time required for execution decreases, and the quality of the results improves considerably.



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Figure 6. Mesh configurations used in solving two-dimensional anisotropic problem.

Here we would like to reiterate the fact that owing to the iterative approach used in our work, there is no need to renumber the nodes and elements while modifying the mesh from that in Figure 6B to that in Figure 6C; the mesh configuration can be modified locally merely by adding or changing a few cards in the original data deck.

Example 3: The third example is devoted to a non-uniform region with complex anisotropy. The governing partial differential equation is

$$K_{xx} \frac{\partial^2 h}{\partial x^2} + 2 K_{xy} \frac{\partial^2 h}{\partial x \partial y} + K_{yy} \frac{\partial^2 h}{\partial y^2} = \frac{\partial h}{\partial t}; \quad 0 \leq x \leq 1;$$

$$0 \leq y \leq 0.8; \quad t \geq 0 \quad (28)$$

subject to the following initial and boundary conditions

$$h(x, y, 0) = 0$$

$$h(1, y, 0) = h(x, 0, t) = 1 \quad (29)$$

$$\frac{\partial h}{\partial x}(0, y, t) = \frac{\partial h}{\partial y}(x, 0.8, t) = 0$$

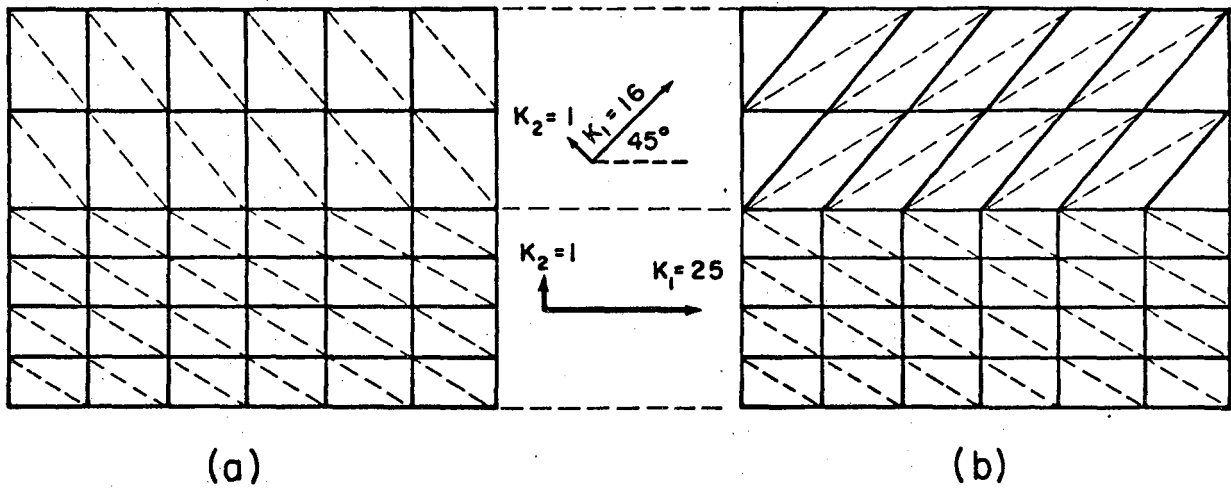
The lower half of the flow region has principal conductivities $K_1 = 25$ and $K_2 = 1$ oriented parallel to the coordinates, as shown in Figure 7. The upper half has principal conductivities $K_1 = 16$ and $K_2 = 1$ oriented at a 45° angle relative to the coordinates. The mixed derivative in (28) arises from the inclined orientation of the principal conductivities in the upper region.

The purpose of this example is to illustrate our method of constructing a finite element mesh for a complex anisotropic system in a manner that will ensure diagonal dominance. Figure 7A shows a rectangular mesh in

which each rectangle is subdivided into two triangles along a NW-SE direction. This mesh does not lead to a diagonally dominant matrix because if we contract the upper region by a factor of 4 parallel to the direction of $K_1 = 16$, we obtain triangles with large obtuse angles. If the rectangles are subdivided into triangles along a NE-SW direction, contracting the mesh parallel to K_1 will still lead to relatively large obtuse angles.

The way to overcome the difficulty is to (a) contract the upper region by a factor of 4 parallel to K_1 , (b) construct a mesh without obtuse angles in the transformed domain, and (c) expand this mesh to the original anisotropic domain, as shown in Figure 8. The complete mesh is depicted in Figure 7B and FLUMP indicates that the resulting matrix $[\underline{\lambda}]$ is indeed diagonally dominant at each node.

The problem was solved with the mixed explicit-implicit method using both meshes in Figure 7. The results were quite different from each other and, in the absence of an analytical solution to serve as a check on the accuracy of the numerical solution, we can only suspect that the results obtained with the mesh in Figure 7B are more accurate than those obtained with the rectangular mesh. However, there is little doubt about the superiority of the mesh in Figure 7B when execution times are compared: With this mesh, $t = 0.1$ was reached in 34 time steps, 431 iterations, and 0.903 seconds of execution time on the CDC 7600. With the rectangular mesh in Figure 7A the same time was reached in 39 time steps and 571 iterations, requiring 1.708 seconds for execution (i.e., nearly double the time required with the inclined mesh).



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Figure 7. Mesh configurations used in solving complex anisotropic problem.

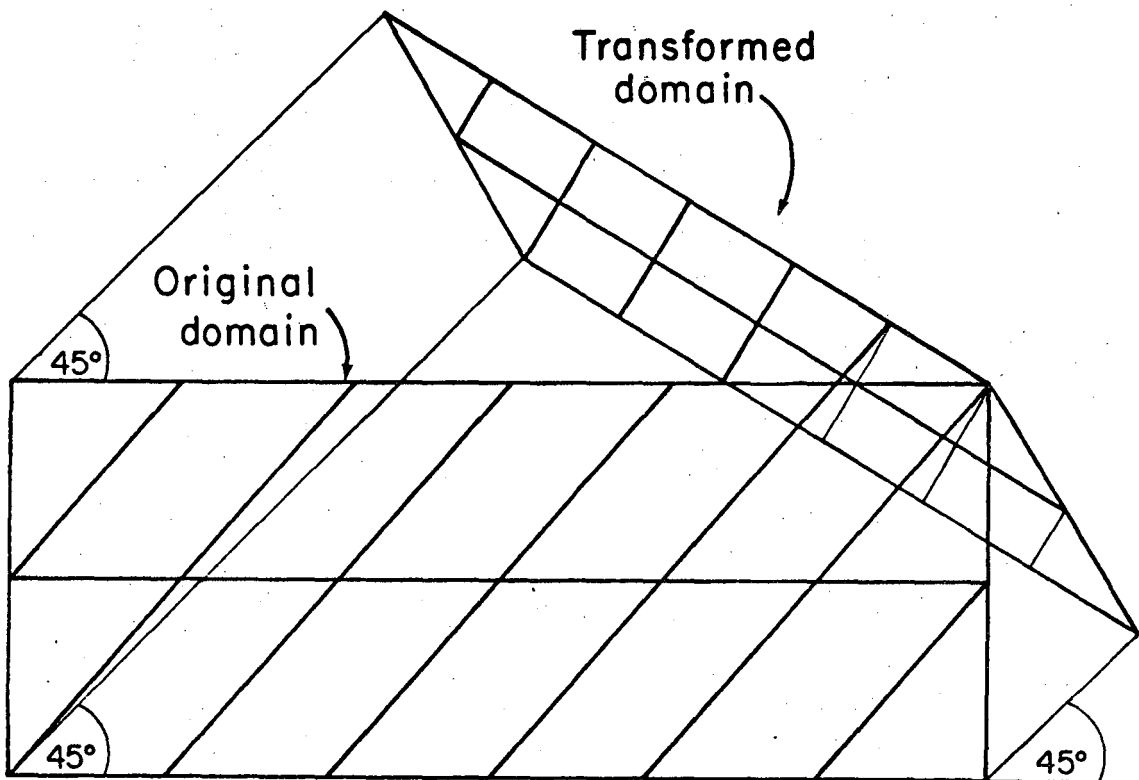


Figure 8. Transformation of upper anisotropic segment into equivalent isotropic domain.

Conclusions

1. The mixed explicit-implicit iterative finite element scheme proposed in this work has been implemented in a computer program entitled FLUMP. The program can conveniently treat two-dimensional and axisymmetric problems involving non-uniform regions with complex geometry and arbitrary anisotropy. Quasilinear problems can also be handled.

2. The mixed explicit-implicit approach is especially well suited for problems that might otherwise involve matrices with large band widths, problems in which the boundary conditions or forcing functions vary often and rapidly with time, problems characterized by a significant spatial variability of element sizes and material properties, and quasilinear problems in which the coefficients vary with the dependent variable.

3. The performance of the mixed explicit-implicit scheme is strongly affected by the way in which the finite element mesh is constructed.

4. If the finite element mesh is constructed in a manner that leads to a diagonally dominant $[\underline{\lambda}]$ matrix, then the mixed scheme is capable of yielding highly accurate results. The mixed scheme can achieve a high degree of accuracy by requiring a lesser amount of computer time than other explicit or iterative implicit methods.

5. By following a few simple guidelines, one can always construct a finite element mesh that results in a diagonally dominant $[\underline{\lambda}]$ matrix.

Acknowledgment

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Table IV: Deviation of mixed explicit-implicit results
at $t = 0.002$ from analytical solution in Table II.

A. Using mesh in Figure 6A.

.022	-.026	-.079	-.053	.228	0
-.003	-.054	-.087	.048	.387	
.019	-.027	-.078	-.053	.216	0
-.005	-.052	-.083	.040	.350	
.013	-.028	-.073	-.052	.180	0
-.010	-.049	-.075	.024	.277	
.006	-.028	-.062	-.047	.126	0
-.014	-.043	-.060	.006	.175	
-.005	-.028	-.048	-.039	.058	0
-.018	-.033	-.039	-.013	.054	
0	0	0	0	0	0

B. Using mesh in Figure 6B.

-.007	-.011	-.013	-.003	-.085	0
-.012	-.015	-.011	-.046	.231	
-.008	-.013	-.015	-.007	-.063	0
-.014	-.017	-.014	-.042	.176	
-.011	-.017	-.018	-.013	-.048	0
-.017	-.021	-.019	-.039	.116	
-.013	-.021	-.022	-.019	-.037	0
-.019	-.024	-.022	-.034	.061	
-.014	-.025	-.025	-.024	-.030	0
-.018	-.024	-.024	-.027	.011	
0	0	0	0	0	0

Table V: Deviation of mixed explicit-implicit results
at $t = .01$ from analytical solution in Table II.

A. Using mesh in Figure 6A.

-.017		-.025		-.022		.001		.031		0
	-.021		-.025		-.013		.018		.025	
-.016		-.024		-.021		.001		.029		0
	-.020		-.023		-.012		.016		.022	
-.015		-.021		-.019		0		.025		0
	-.017		-.020		-.011		.012		.018	
-.012		-.017		-.015		-.001		.017		0
	-.012		.006		.014		.027		.011	
-.008		-.011		-.010		-.002		.008		0
	-.006		-.008		-.005		0		.003	
0		0		0		0		0		0

B. Using mesh in Figure 6B.

-.012		-.015		-.015		-.018		-.016		0
	-.013		-.015		-.016		-.013		.002	
-.011		-.014		-.015		-.016		-.014		0
	-.013		-.014		-.015		-.012		.001	
-.010		-.013		-.014		-.014		-.012		0
	-.011		-.012		-.012		-.008		0	
-.008		-.011		-.011		-.012		-.010		0
	-.008		-.009		-.010		-.009		0	
-.006		-.008		-.008		-.008		-.007		0
	-.004		-.005		-.006		-.004		-.001	
0		0		0		0		0		0

Table V (continued)

C. Using mesh in Figure 6C.

-.009	-.009	-.010	-.010	-.010	-.009	-.010	-.008	-.008	-.006	0
	-.009		-.010		-.009		-.008		-.005	
-.008		-.009		-.009		-.009		-.007		0
	-.009		-.009		-.009		-.008		-.005	
-.008		-.009		-.009		-.008		-.006		0
	-.008		-.008		-.008		-.006		-.004	
-.006		-.007		-.007		-.007		-.006		0
	-.005		-.006		-.006		-.005		-.003	
-.004		-.005		-.005		-.005		-.004		0
	-.003		-.003		-.003		-.003		-.002	
0	0	0	0	0	0	0	0	0	0	0

Table VI. Comparison of performance
using three difference meshes.

<u>Using mesh in Figure</u>	<u>Number of time steps to t = 0.04</u>	<u>Number of iterations to t = 0.04</u>	<u>Execution time in seconds</u>
6A	79	984	5.442
6B	37	329	1.091
6C	36	332	1.192

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