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EXTENSION OF THE CRANK-NICHOLSON PROCEDURE TO A CLASS OF INTEGRODIFFERENTIAL EQUATIONS

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Abstract

The Crank-Nicholson procedure is widely used as a step by step integration technique for ordinary differential equations. The application of this procedure to integro-differential equations, however, is not straight forward. This paper gives an extension of the Crank-Nicholson procedure to a class of integrodifferential equations with a singular kernel. As an example, the method is applied to the integro-differential equations of groundwater hydrology.

1. Introduction

The Crank-Nicholson procedure is widely used as a step by step integration technique for ordinary differential equations. However, the application of this procedure to a system of integrodifferential equations such as

$$\underset{\approx}{a}\frac{d\underset{\sim}{u}}{dt} = \underset{\approx}{B}\underset{\sim}{u}(t) + \underset{\approx}{C}\int_0^t \underset{\approx}{g}(t-\tau)\frac{d\underset{\sim}{u}}{dt}(\tau)d\tau + \underset{\sim}{D}$$

is not straight forward, because:

1) The derivative frequently cannot be expressed explicitly in terms of the function itself.
2) The kernel or memory function is often singular.
3) The characteristic time of the solution is unrelated to the characteristic time of the memory function. Therefore, it is important to use approximations which do not involve the latter, in order that the length of the time step Δt be limited by the characteristic time of the solution only.
4) It is difficult to handle the integral terms efficiently without greatly increasing both processor and memory requirements.

This paper gives a way of treating this problem for a class of integrodifferential equations whose kernel may be singular.

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The basic features of this method are:

a) The solution at time $t+\Delta t$ is expressed in terms of the solution at time t with an error of order $o(\Delta t^3)$ which is independent of the characteristic time of the memory.

b) The memory function is treated in an exact manner in the interval $[t, t+\Delta t]$. Thus, the singularity of the kernel is properly handled and at the same time the accuracy of the method remains independent of the characteristic time of the memory function.

c) When the kernel of the equation can be represented by a series of exponential functions:

$$\underset{\approx}{g}(t) = \sum_{n=1}^{\infty} \underset{\approx}{a}_n e^{-\alpha_n t}$$

the integral terms can be evaluated without recourse to past values of the solution. Hence, memory and processor requirements are greatly reduced.

The integrodifferential equation approach to groundwater flow [Herrera, 1976] gives rise to a system of partial integro differential equations. As an example, using the finite element method, this system is transformed into one of the type here discussed, where g is the scalar function

$$g(t) = 2 \sum_{n=1}^{\infty} e^{-n^2\pi^2 t} = (\pi t)^{-1/2}(1+2 \sum_{n=1}^{\infty} e^{-n^2/t})-1$$

In previous work [Herrera et al., 1976; Herrera and Yates, 1977] the resulting system of equations was approximated to make it susceptible for numerical treatment. The method developed in this paper represents an improvement in that the equations can be handled without modification, achieving greater accuracy and reducing both memory requirements and processor time. These results have been confirmed by comparative runs.

2. Extension of the Crank-Nicholson procedure

Consider the equation

$$\underset{\approx}{A} \frac{d\underset{\sim}{u}}{dt} = \underset{\approx}{B}\, \underset{\sim}{u}(t) + \underset{\approx}{C} \int_0^t \underset{\approx}{g}(\tau) \frac{d\underset{\sim}{u}}{dt}(t-\tau)\,d\tau + \underset{\sim}{D} \qquad (1)$$

The first step in applying the standard Crank-Nicholson procedure involves the evaluation of equation (1) at $t+\Delta t/2$ using the approximations

$$\underset{\sim}{u}(t+\Delta t/2) = \frac{\underset{\sim}{u}(t+\Delta t)+\underset{\sim}{u}(t)}{2} + o(\Delta t^2) \qquad (2a)$$

$$\frac{d\underset{\sim}{u}}{dt}(t+\Delta t/2) = \frac{\underset{\sim}{u}(t+\Delta t)-\underset{\sim}{u}(t)}{\Delta t} + o(\Delta t^2) \tag{2b}$$

Substitution of these expressions in (1) yields

$$\underset{\approx}{a}\frac{\underset{\sim}{\Gamma}(t)}{\Delta t} = \underset{\approx}{B}(\underset{\sim}{u}(t)+\tfrac{1}{2}\underset{\sim}{\Gamma}(t)) + \underset{\approx}{C}\,\underset{\sim}{\sigma}(t+\Delta t/2)+\underset{\sim}{\mathcal{D}}+o(\Delta t^2) \tag{3}$$

where

$$\underset{\sim}{\Gamma}(t) = \underset{\sim}{u}(t+\Delta t) - \underset{\sim}{u}(t) \quad ; \tag{4}$$

and

$$\underset{\sim}{\sigma}(t+\Delta t/2) = \int_o^{t+t/2} \underset{\approx}{g}(\tau)\frac{d\underset{\sim}{u}}{dt}(t+\Delta t/2-\tau)\,d\tau \tag{5}$$

Since

$$\underset{\sim}{\sigma}(t+\Delta t/2) = \int_o^{t} \underset{\approx}{g}(t+\Delta t/2-\tau)\frac{d\underset{\sim}{u}}{dt}(\tau)\,d\tau + \int_o^{\Delta t/2} \underset{\approx}{g}(\tau)\frac{d\underset{\sim}{u}}{dt}(t+\Delta t/2-\tau)\,d\tau \tag{6}$$

and

$$\frac{d\underset{\sim}{u}}{dt}(t+\Delta t/2-\tau) = \frac{d\underset{\sim}{u}}{dt}(t+\Delta t/2)+\frac{1}{\Delta t}\frac{d\underset{\sim}{u}}{dt}(t-\frac{\Delta t}{2})-[\frac{d\underset{\sim}{u}}{dt}(t+\frac{\Delta t}{2})]\tau+o(\Delta t^2) \tag{7}$$

it follows that

$$\int_o^{\Delta t/2} \underset{\approx}{g}(\tau)\frac{d\underset{\sim}{u}}{dt}(t+\Delta t/2-\tau)\,d\tau = [\int_o^{\Delta t/2}(1-\frac{\tau}{\Delta t})\underset{\approx}{g}(\tau)\,d\tau]\frac{d\underset{\sim}{u}}{dt}(t+\Delta t/2)$$
$$+[\int_o^{\Delta t/2}\frac{\tau}{\Delta t}\,\underset{\approx}{g}(\tau)\,d\tau]\,\frac{d\underset{\sim}{u}}{dt}(t-\Delta t/2)+o(\Delta t^2) \tag{8}$$

Writing

$$\underset{\sim}{S}(t) = \int_o^{t} \underset{\approx}{g}(t+\Delta t/2-\tau)\frac{d\underset{\sim}{u}}{dt}(\tau)\,d\tau \tag{9a}$$

$$\underset{\approx}{Q}(t) = \int_o^{t/2}(1-\tau/t)\,\underset{\approx}{g}(\tau)\,d\tau \tag{9b}$$

$$\underset{\approx}{R}(t) = \int_o^{t/2}\frac{\tau}{t}\,\underset{\approx}{g}(\tau)\,d\tau \tag{9c}$$

equation (3) yields by means of (2) and (4).

$$[\underset{\approx}{a}-\underset{\approx}{C}\underset{\approx}{G}(\Delta t) - \underset{\approx}{B}\Delta t/2]\underset{\sim}{\Gamma}(t) = [\underset{\approx}{B}\underset{\sim}{u}(t)+\underset{\approx}{C}\underset{\sim}{S}(t)]\Delta t+\underset{\approx}{C}\underset{\approx}{R}(\Delta t)\underset{\sim}{\Gamma}(t-\Delta t)$$
$$+\underset{\sim}{\mathcal{D}}\Delta t + o(\Delta t^3) \tag{10}$$

This last equation constitutes a recursive scheme of third order in Δt similar to the Crank-Nicholson procedure. The

functions $\underset{\sim}{G}(\Delta t)$ and $\underset{\sim}{R}(\Delta t)$ are well-defined even if $\underset{\sim}{g}(\tau)$ is singular at $\tau=0$, provided this function is integrable.

3. Application to ground-water hydrology

There are some difficulties that hinder the direct use of the extension of the Crank-Nicholson procedure to integro-differential equations. If equation (10) , as it stands were to be solved numerically step by step in time, it would be necessary to evaluate the convolution term (9a) at each step. To this end, one could use the exact values of the function $\underset{\sim}{g}$. However, if this were done, it would be necessary to carry out the integration from zero to t anew on each step, since the integrand depends on t, which is being changed. This is inconvenient for two reasons: first, the number of computations required would increase beyond reasonable limits, and second, it would be necessary to keep at hand the entire past history of $d\underset{\sim}{u}/dt$. Thus, the memory requirements of the computer would be greatly increased.

A case for which these difficulties can be removed is when the memory function $\underset{\sim}{g}$ can be approximated by a series of exponentials. The ideas behind the procedure are not complicated and will not be discussed in their greatest generality; instead, they will be illustrated by means of an example taken from Ground Water Hydrology.

The transient behavior of a single leaky aquifer with axial symmetry is governed by the integrodifferential equation [Herrera and Rodarte, 1973; Herrera, 1974; Herrera et al., 1976; Herrera and Yates, 1977]:

$$\frac{\partial^2 s}{\partial r^2} + \frac{1}{r}\frac{\partial s}{\partial r} - s - g \star \frac{\partial s}{\partial t} = \frac{1}{\alpha}\frac{\partial s}{\partial t} \; ; \; r \text{ and } t>0 \qquad (11)$$

subject to suitable boundary and initial conditions. The variables used in (11) are dimensionless, the star stands for convolution, and g is

$$g(t) \equiv 2\sum_{n=1}^{\infty} e^{-n^2\pi^2 t} = (\pi t)^{-1/2}\left(1+2\sum_{n=1}^{\infty} e^{-n^2/t}\right)-1 \qquad (12)$$

A discussion of the physical meaning of equation (11), is given in the above mentioned papers.

Equation (11) can be transformed into a system of integrodifferential equations in the single variable t by application of the finite element method [Herrera et al., 1976; Herrera and Yates, 1977]. As usual, the infinite interval $[0,\infty)$ will be approximated by the finite interval $[0,R]$, where R is taken sufficiently large. A finite element mesh is assumed to cover $[0,R]$ and the basis function $\psi_i(r)$, $i=1,\ldots,N'$, are defined there. The approximate solution of (11), is

$$s(r,t) = \sum_{n=1}^{N'} p_i(t)\psi_i(r) \tag{13}$$

where $\underset{\sim}{P}(t)=(p_1,\ldots,p_{N'})$ satisfies the system of integro-differential equations in the single variable t:

$$\frac{1}{\alpha}\underset{\approx}{M}\frac{\partial \underset{\sim}{P}}{\partial t}(t) = -(\underset{\approx}{K}+\underset{\approx}{M})\underset{\sim}{P}(t) - \underset{\approx}{M}\int_o^t g(\tau)\frac{\partial \underset{\sim}{P}}{\partial t}(t-\tau)d\tau + \underset{\sim}{C} \tag{14}$$

where

$$M_{ij} = \int_o^R r\psi_i(r)\psi_j(r)dr \tag{15a}$$

$$K_{ij} = \int_o^R r\psi_i'(r)\psi_j'(r)dr \tag{15b}$$

$$C_i = \frac{Q}{2\pi T}\psi_i(0) \tag{15c}$$

Equation (14) is derived by applying the Garlekin procedure to equation (11) [see Herrera and Yates, 1977].

Application of the extension of the Crank-Nicholson formula (10) to (14) leads to

$$[\frac{1}{\alpha}\underset{\approx}{M}+G(\Delta t)\underset{\approx}{M} + (\underset{\approx}{K}+\underset{\approx}{M})\Delta t/2]\underset{\sim}{\Gamma}(t) = -[(\underset{\approx}{K}+\underset{\approx}{M})\underset{\sim}{P}(t)+\underset{\approx}{M}\underset{\sim}{S}(t)]\Delta t$$
$$- R(\Delta t)\underset{\approx}{M}\underset{\sim}{\Gamma}(t-\Delta t) + \underset{\sim}{C}\Delta t + o(\Delta t^3) \tag{16}$$

where G(t) and R(t) are scalar functions related to the scalar function g(t), by equations (9b,c). Setting

$$\underset{\approx}{A} = [\frac{1}{\alpha} + \frac{\Delta t}{2} + \underset{\approx}{G}(\Delta t)]\underset{\approx}{M} + \frac{1}{2}\underset{\approx}{K}\Delta t \tag{17a}$$

$$\underset{\approx}{B} = -(\underset{\approx}{K}+\underset{\approx}{M})\Delta t \tag{17b}$$

equation (16) can be rewritten as

$$\underset{\approx}{A}\underset{\sim}{\Gamma}(t) = \underset{\approx}{B}\underset{\sim}{P}(t) - \underset{\approx}{M}\underset{\sim}{S}(t)\Delta t - R(\Delta t)\underset{\approx}{M}\underset{\sim}{\Gamma}(t-\Delta t)+\underset{\sim}{C}\Delta t+o(\Delta t^3) \tag{18}$$

4. Approximation of the kernel function

To compute

$$\underset{\sim}{S}(t) = \int_o^t g(t+\frac{\Delta t}{2} - \tau)\underset{\sim}{P}'(\tau)d\tau \tag{19}$$

which occurs in (18), the approximation

$$g(t) \approx g_N(t) = 2\sum_{n=1}^{N} e^{-n^2\pi^2 t} + a_N\,\delta(t-\Delta t) \tag{20}$$

will be used. Here

$$a_N = 2 \sum_{n=N+1}^{\infty} \frac{e^{-n^2\pi^2\Delta t/2}}{n^2\pi^2} \qquad (21)$$

This approximation is motivated by one that has been successfully used in ground-water hydrology [Hantush, 1960; Herrera and Rodarte, 1973], and has been more thoroughly discussed in previous work [Herrera et al., 1976; Herrera and Yates,1977]. The constant a_N is chosen so that

$$\int_{\Delta t/2}^{\infty} g(t)dt = \int_{\Delta t/2}^{\infty} g_N(t)dt. \qquad (22)$$

Including the delta function has the effect of incorporating at $t-\Delta t/2$ the integral of the terms neglected in the infinite series.

With this approximation, equation (19) becomes

$$\underset{\sim}{S}(t) = 2 \sum_{n=1}^{N} e^{-n^2\pi^2\Delta t/2} \underset{\sim}{D}_n(t) + a_N \underset{\sim}{P}'(t-\Delta t/2) \qquad (23)$$

where

$$\underset{\sim}{D}_n(t) = e^{-n^2\pi^2 t} \int_o^t \underset{\sim}{P}'(\tau) e^{n^2\pi^2\tau} d\tau \qquad (24)$$

The values of $\underset{\sim}{D}_n(t)$ can be updated without recourse to past values, because

$$\underset{\sim}{D}_n(t+\Delta t) = e^{-n^2\pi^2\Delta t} \underset{\sim}{D}_n(t) + e^{-n^2\pi^2(t+\Delta t)} \int_t^{t+\Delta t} \underset{\sim}{P}'(\tau) e^{n^2\pi^2\tau} d\tau \qquad (25)$$

The last integral can be evaluated using the linear interpolation

$$\underset{\sim}{P}(t+\Delta t-\tau) = \underset{\sim}{P}(t+\Delta t) - \frac{\underset{\sim}{\Gamma}(t)}{\Delta t}\tau + o(\Delta t^2) \; ; \; 0 \leq \tau \leq \Delta t \qquad (26)$$

In this manner, it is obtained

$$\int_t^{t+\Delta t} \underset{\sim}{P}'(\tau) e^{n^2\pi^2\tau} d\tau = \frac{e^{n^2\pi^2 t}}{n^2\pi^2\Delta t} \underset{\sim}{\Gamma}(t)[e^{n^2\pi^2\Delta t} - 1] + o(\Delta t^3) \qquad (27)$$

Consequently

$$\underset{\sim}{D}_n(t+\Delta t) = e^{-n^2\pi^2\Delta t} \underset{\sim}{D}_n(t) + \frac{\underset{\sim}{\Gamma}(t)}{n^2\pi^2\Delta t}(1-e^{-n^2\pi^2\Delta t}) + o(\Delta t^3) \qquad (28)$$

which is the desired formula. In view of this result equation (23) can be written as

$$\underset{\sim}{S}(t) = 2 \sum_{n=1}^{N} e^{-n^2\pi^2\Delta t/2} \underset{\sim}{D}_n(t) + a_N \frac{\underset{\sim}{\Gamma}(t-\Delta t)}{\Delta t} + o(\Delta t^3) \qquad (29)$$

Finally, equation (18) becomes

$$\underset{\sim}{A}\underset{\sim}{\Gamma}(t) = \underset{\sim}{B}\underset{\sim}{P}(t)-\underset{\sim}{M}\{2\sum_{n=1}^{N} e^{-n^2\pi^2\Delta t/2}\underset{\sim}{D}_n(t)\Delta t+[a_N+R(\Delta t)]\underset{\sim}{\Gamma}(t-\Delta t)\}$$

$$+ \underset{\sim}{C}\Delta t + o(\Delta t^3) \qquad (30)$$

Equations (28) and (30) provide a recursive procedure of third order in Δt (i.e. giving the solution to second order) which can be applied directly, because the value of $\underset{\sim}{S}(t)$ has been eliminated by means of (29) and $\underset{\sim}{D}_n$ can be updated using (28).

5. Discussion

When treating numerically a system of integrodifferential equations of the type here discussed (equation 1), it is necessary to approximate the kernel $\underset{\sim}{g}(t)$ in some way; otherwise it would be necessary to compute the integral terms in the interval (0,t) anew on each step. This would greatly increase processor and memory requirements. When the kernel can be approximated by a finite exponential series this difficulty is overcome. However, if $\underset{\sim}{g}(t)$ is singular at t=0, the exponential series is a poor approximation there. The extension of the Crank-Nicholson procedure presented here allows an exact treatment of the kernel in a neighborhood of the singularity.

It should be observed that when the kernel is singular, it is not possible to apply integration by parts in order to express the integral occurring in equation (1), in terms of the function u. This is because g'(t) is not integrable in a neighbourhood of zero. Our method permits the derivative to be expressed directly in terms of the function itself.

Frequently, the characteristic time of the solution corresponding to a given problem can be much larger than the characteristic time of the kernel function. One advantage resulting from the exact treatment of the kernel function $\underset{\sim}{g}$, is that the size of the time steps Δt, is limited only by the length of the characteristic time of the solution.

The number N of terms required in the series expansion (20), to achieve a given accuracy, depends on the time step Δt, which in turn is determined by the characteristic time of the solution. A method was previously developed [Herrera and Yates, 1977] which is based in approximating the integrodifferential equations themselves. For such a method a rule was given relating N with Δt. In comparative runs it has been found that the present method permits reducing N considerably; this implies an important reduction of memory requirements and processor time.

References

1. Hantush, M.S., "Modification of the theory of leaky aquifers," J. Geophys. Res., 65 (11), 1960, p.p. 3713-3725.

2. Herrera, I., "Integrodifferential equations for systems of leaky aquifers and applications. Part 2. Error analysis of approximate theories," Water Resources Research, 10 (4), 1974, p.p. 811-820.

3. Herrera, I., "A review of the integrodifferential equations approach to leaky aquifer mechanics," invited paper published 1976 AWRA Symposium Proceedings Advances in Groundwater Hydrology, 1976.

4. Herrera, I., and Rodarte, L., "Integrodifferential equations for systems of leaky aquifers and applications. Part 1. The nature of approximate theories," Water Resources Research, 9 (4), 1973, p.p. 995-1005.

5. Herrera, I., et al., "A family of approximate numerical procedures for leaky aquifer systems," Proc. Second International Symposium on Finite Element Methods in Flow Problems, S. Margherita Ligure, Italy, 1976, p.p. 355-364.

6. Herrera, I., and Yates, R., "Integrodifferential equations for systems of leaky aquifers and applications. Part 3. A numerical method of unlimited applicability," Water Resources Research, 13 (4), 1977.

GENERALIZATION OF FINITE ELEMENT ALTERNATING-DIRECTION TECHNIQUES TO NON-RECTANGULAR REGIONS

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Summary

A convergent finite element alternating-direction procedure is presented for solving the heat equation on non-rectangular regions in $\mathbb{R}^2$. This procedure is unconditionally stable in time and has the following advantages:

(1) The matrix which must be inverted is independent of time, so it need only be decomposed one time.

(2) The matrix which must be inverted can be factored into the product of two matrices, each of which corresponds to the solution of one-dimensional problems.

A key concept in this procedure is that we can approximate the Jacobian of a certain transformation, locally on patches of elements, by a function which can be factored into a function of x times a function of y.

1. Introduction

For simplicity, we limit this discussion to the heat equation

$$u_t(\underset{\sim}{\xi},t) - \nabla\cdot(k\nabla u(\underset{\sim}{\xi},t)) = f(\underset{\sim}{\xi},t), \quad (\underset{\sim}{\xi},t) \in \Omega_g \times (0,T], \tag{1}$$

with boundary conditions

$$u(\underset{\sim}{\xi},t) = 0, \quad (\underset{\sim}{\xi},t) \in \partial\Omega_g \times (0,T]$$

$$u(\underset{\sim}{\xi},0) = u_0(\underset{\sim}{\xi}).$$

Extensions of these results to $\mathbb{R}^3$ and to more general nonlinear parabolic and hyperbolic problems are briefly mentioned at the conclusion of this paper. For a more complete discussion the reader is referred to Hayes [4].

The Galerkin formulation of equation (1) is given by Oden and Reddy [5],

$$(U_t,V)_{\Omega_g} + (k\nabla U,\nabla V)_{\Omega_g} = (f,V)_{\Omega_g}, \quad V \in S_h(\Omega_g), \tag{2}$$

where $(f,g)_{\Omega_g} = \int_{\Omega_g} fg\,d\xi$, and $S_h(\Omega_g)$ is a finite dimensional subspace of $H_0^1(\Omega_g)$.

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The relatively large values of the standard deviation is only partially due to the error of the measurements (5%). Instead, the experimental results prove that, apart from the solutions obtained with the assumption CR = 0 (equation 14 : discharge condition) other roll-waves can exist in the channel, which individually do not convey the correct discharge Q, provided that the mean discharge over several different waves equals the (constant) discharge Q, supplied to the channel. This result did not follow from the theory by Brock [3] but the large "measurement errors" he mentioned (up to 100 %) can be explained by the above theory.

6. Conclusions

The integration of the non-linear momentum-equation yields, for given values of Re and F, an infinity of possible roll-wave solutions for each value of the maximum wave-depth. One of these solutions has an infinite wave-length. The exact solution can be approximated by the cnoïdal wave theory. These results are in good agreement with the experiments.

References

1. Berlamont, J., "Roll-waves". (Rolgolven). Thesis presente to the Ghent State University, Ghent, Belgium, in partial fulfilment of the requirements for the Doctor's degree in engineering. 1975. (In Dutch).

2. Berlamont, J., "Roll-waves in inclined rectangular open channels," Int. Symposium on Unsteady flow in open channels, Univ. of Newcastle-upon-Tyne, U.K., 12-15 April 1976.

3. Brock, R.R., "Development of roll-wave trains in open channels," Journal of the Hydraulics Division, A.S.C.E., Vol. 95, n° HY4, 1969, p.p. 1401-1427.

4. Dressler, R.F., "Mathematical solution of the problem of roll-waves in inclined open channels, "Communications on pure and applied mathematics," N.Y., Vol. 2, n° 2-3, 1949, p.p. 149-194.

5. Laitone, E.V., "Limiting conditions for cnoïdal and stokes waves," Journal of geophysical research, Vol. 67, n° 4, April 1962, p.p. 1555-1564.

6. Ralston, "Mathematical methods for digital computers," J. Wiley and Sons, New York, 1960, p.p. 95-109.

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