MODELLING GROUND-WATER FLOW WITH THE GLOBAL AND FINITE ELEMENT METHODS

J.F. Botha and G.N. Bakkes

Institute for Ground-water Studies
University of the Orange Free State, Bloemfontein

INTRODUCTION

The two numerical methods most frequently used to solve differential equations arising in science and engineering are perhaps the finite difference (FDM) and finite element (FEM) methods. The basic philosophy behind both these methods is to replace the true solution by an approximate one constructed from a suitable set of basis functions. In the case of the FEM the basis functions are usually selected from the set of piecewise continuous polynomials, while the FDM is based on interpolation polynomials [Botha and Pinder (1983)]. This reduces the problem to the simple operation of solving a set of equations

$$F(c) = 0$$

for the expansion coefficients c in the approximating series.

A major disadvantage of both the methods is that, due to the well-known Runge-Meray phenomenon [Stroud (1974)], only low order polynomials can be used. To improve their accuracy, the number of polynomial pieces, i.e. the number of expansion coefficients has to be increased. Such a refinement requires that the domain of interest be discretised anew, a process that can be quite time-consuming, in particular when studying the convergence rate of these methods.

There exist methods whose accuracy can be improved without rediscretising the domain of interest. Such methods use elementary functions that have global support, hence the name global methods.

Global methods have in general some serious limitations, the best known of which is the difficulty to apply them on domains with irregular boundaries. This can, however, be circumvented by using transfinite interpolation [Gordon and Hall (1973)]. Another difficulty is that it is sometimes advantageous to discretise the domain in a number of subdomains. As all the presently known global methods are based on either a variational principle or the method or the method of weighted residuals [Finlayson (1972)], this may prove not to be easy.

The reason for this is not so much connected with the methods themselves, but rather with the restrictions placed on the admissible basis functions. This aspect will be dealt with more fully in the next section where it will be shown how these restrictions can be removed. The paper will then proceed with the global variational method recently introduced by Delves and his co-workers [Delves and Hall (1979), Delves and Freeman (1981)], for elliptic type problems. It will then be shown how the method can be extended to multiple domains and parabolic equations. The method will be finally applied to a few problems from the field of geohydrology and the results compared with those obtained from the FEM.

THE RAYLEIGH-RITZ AND GLOBAL VARIATIONAL METHODS

The Rayleigh-Ritz method (RRM) is, as is well-known, particularly useful for solving elliptic type problems [Oden and Reddy (1976)] such as

$$Au = -\nabla [p \nabla u] + qu = f$$

defined over a closed domain Ω with boundary $\partial \Omega$ where ∇ is the usual gradient operator. Let C_1 and C_2 be two non-overlapping segments of this boundary and assume that Equation 1 is subject to the Dirichlet boundary condition

$$u(\underline{x}) = g(\underline{x}) \qquad \underline{x} \in C_1$$

and the mixed boundary condition

$$p \nabla u \cdot \underline{n} = b(\underline{x})u(\underline{x}) + h(\underline{x}) \cdot \underline{x} \in C_2$$

with \underline{n} the unit normal vector on C_2 . If the boundary C_1 is sufficiently large, this problem has a unique solution [Delves and Hall (1979)]

$$\mathbf{u}(\mathbf{x}) \in \mathbf{H}^1(\mathbf{\Omega})$$

where H¹ denotes the Hilbert space with first derivatives continuous.

To solve this problem by the RRM, one first selects a set of suitable basis functions $\{v_i\}_0^n$, approximates the true solution u by a trial function

$$\mathbf{w} = \sum_{i=0}^{n} c_i \mathbf{v}_i$$

and then minimizes the functional

$$F[w] = (Aw,w) - 2(f,w)_2$$

where

$$(Aw,w) = \int_{\Omega} Awwd\Omega$$
 and $(f,w)_2 = \int_{\Omega} fwd\Omega$

This is equivalent to seeking the function w such that [Oden and Reddy (1976)]

$$(Aw,w) = (f,w)_2$$

In the case of the operator A defined in Equation 1, application of Green's theorem to the left-hand side of Equation 6 yields

$$\int [p \nabla w \nabla v_i + qwv_i] d\Omega = \int_{\Omega} fv_i d\Omega + \int_{\partial \Omega} v_i p \nabla w \cdot \underline{n} ds$$
 7

If ∇ w in the line integral on the right-hand side of Equation 7 is known, then this equation represents a system of linear equations for the coefficients c_i of Equation 5.

This is clearly the case for the mixed boundary condition where ∇ w can simply be replaced by its equivalent expression from Equation 3. The set of basis functions used with mixed boundary values thus need not satisfy any constraints. This is not possible in the case of a Dirichlet condition.

The method most often employed with a Dirichlet condition is to replace the trial function in Equation 4, by another one of the form

$$w = g + \sum_{i=1}^{n} c_i v_i$$

where the v_i now have to satisfy homogeneous Dirichlet boundary conditions

$$v_i = 0$$
 on C_1 .

The line integral vanishes in this case and Equation 6 reduces again to a system of linear equations with

$$F_{i} = \int_{\Omega} f v_{i} d\Omega - \int_{\Omega} [p(\nabla g \nabla v_{i}) + qg v_{i}] d\Omega$$

This constraint on the basis functions is rather restricting. It prohibits, for example, the use of many useful elementary functions, e.g. Chebyshev polynomials, as basis functions. Moreover, it does not allow the division of the domain into subdomains, because to impose the continuity condtion, Equation 4, would require a non-homogeneous boundary condition. There exists, however, an alternative approach.

It is well-known that Equation 1 is the Euler-Lagrange equation that minimizes the functional in Equation 6. What is less known, is that it also yields a stationary value for the functional

$$F^*[w] = F[w] + \int_{\Omega} \nabla \cdot \underline{G} d\Omega$$

or after applying Gauss' theorem to the integral containing G

$$F^*[w] = F[w] + \int_{\Omega} \underline{G} \cdot \underline{n} ds$$
 9

where \underline{G} is an arbitrary function of w and its gradient ∇ w [Rund (1973)].

Although Equation 1 does not minimize Equation 8 in general, it can be shown [Rund (1973)] that, if G is chosen in such a way that it satisfies the transversa-

lity conditions [Rund (1973)] associated with Equation 8, then Equation 1 will in fact minimize Equation 8 [Rund (1973), Snyman (1982)]. Hence, if G is chosen to satisfy the boundary conditions of Equation 1 and at the same time the necessary transversality conditions, Equation 9 will be a new variational functional (in the sense of the RRM) for the solution of Equation 1, but one for which the basis functions need not satisfy any boundary conditions. This method is known as the Global Variational Method (GVM) [Delves and Hall (1979)].

The best way to illustrate the GVM is to apply it to Equation 1. The transversality conditions for Equation 9 is, in general, of the form [Snyman (1982), Bakkes (1984)]

$$(\nabla^* L + D_{\mathbf{w}} \underline{G}) \cdot \underline{\mathbf{n}} = 0$$

$$\nabla^* G_{\mathbf{j}} \cdot \underline{\mathbf{n}} = 0 \qquad (\mathbf{j} = 1, 2, 3)$$

where

$$L = (p \nabla w \nabla w + qww) - 2fw$$

is the Lagrangian function corresponding to Equation 1 and ∇^* denotes the gradient operator with ∇w as independent variable.

Consider now the function

$$G = a_1 w^2 + a_2 w$$

defined over the segment C_1 , where a_k (k = 1,2) are constants to be determined. The first transversality condition in Equation 10 yields in this case

$$[(2p+a_1)w]. \underline{n} = 0$$

and the second

$$(a_1w + a_2) = 0$$

From these equations follow that

$$a_1 = -2p \text{ and } a_2 = 2pw$$
 11

There will be consistency between Equation 2 and Equation 11 on the boundary C_1 if the second condition in Equation 11 is replaced by

$$a_2 = 2pg$$

The function G to be used with the Dirichlet boundary condition in Equation 2 is thus completely determined

$$G = -2pw^2 + 2gpw.$$

Proceeding in a similar fashion, it can be shown [Bakkes (1984)] that the mixed boundary condition on segment C_2 will be satisfied, provided that the function G is now chosen as

$$G = -(bw^2 + 2hw)n$$

A variational functional 8, suitable for Equation 1, and for which the basis functions need not satisfy any boundary conditions is thus

$$F^*[w] = \int_{\Omega} [p \nabla w \nabla w + qw^2 - 2fw] d\Omega + 2 \int_{\Omega} (g - w)p \nabla w \cdot \underline{n} ds$$

$$C_1$$

$$-2 \int_{\Omega} [(b/2)w^2 + hw] ds$$

$$C_2$$

$$C_3$$

$$C_4$$

$$C_4$$

$$C_5$$

This is a simplified form of the functional originally introduced by Delves and Hall (1979).

THE GLOBAL ELEMENT METHOD (GEM)

The extension of the GVM to domains divided into subdomains, henceforth also referred to as global elements, is straightforward. To show this, consider the domain Ω associated with Equation 1, but now divided into two subdomains Ω_1 and Ω_2 where (k = 1, 2 cyclically, i.e. k + 1 = 1 if k + 1 > 2) as in Figure 1. A solution of Equation 1 can only be accepted on physical grounds if it is continuous across the interface C. This will be true if it satisfies Equation 4, which implies

$$w_1 = w_2$$
 and $\nabla w_1 = \nabla w_2$ on C

The functional 12, valid for the k-th global element, can thus be expressed, using Equation 13, as

$$\begin{aligned} F_k^* &= \int\limits_{\Omega} \left[p(\nabla w_k)^2 + q(w_k)^2 - 2fw_k \right] d\Omega + 2 \int\limits_{C_1} (g - w_k) p \nabla w_k \cdot \underline{n} ds \\ &- 2 \int\limits_{C_2} \left[(b/2)(w_k)^2 + hw_k \right] ds - \int\limits_{C} (w_k - w_{k+1})(p \nabla w_k \cdot \underline{n}_k \\ &- c_2^k \\ &- p \nabla w_{k+1} \cdot \underline{n}_{k+1}) ds \end{aligned}$$

where C_m^k denotes that part of the boundary C_m which belongs to the k-th global element. This approach is known as the global element method (GEM) [Delves and Hall (1979), Bakkes (1984)].

The GEM and the GVM was introduced above for elliptic type differential equations. However, it can be easily extended to parabolic problems. Take for example the parabolic problem

$$D_t u(\underline{x}, t) = a \nabla^2 u(\underline{x}, t) + f$$

where $(\underline{x},t) \in \Omega \otimes [0,T]$ with Ω the same domain as in Equation 1. The functions a and f can in general be functions of \underline{x} , t, u and ∇u . To simplify the notation, this dependence of a and f as well as that of u will be suppressed unless required for reasons of clarity.

The boundary conditions will again be taken to be of the form as defined in Equations 2 and 3, while the initial condition is assumed to be given by

$$u(\underline{x},0) = u_0(\underline{x}).$$

By using linear Lagrange polynomials in time and collocation, [Botha (1982)] was able to show that Equation 14 can always be approximated, correct to the second order in time, by the modified Helmholtz equation

$$\nabla^2 u' - m^2 u' = F(\underline{x}, t^*)$$
 15

where, with u^n the approximation for $u(x,t^n)$, at $t=t^n$

$$u' = u^{n+1} - u^n$$

$$F = -(1/\lambda)[(a/2 - \lambda) \nabla^2 u^{n+1} + (a/2 + \lambda) \nabla^2 u^n + f^{n+1/2}]$$

$$m^2 = [1/(\lambda \Delta t)] \qquad (\Delta t = t^{n+1} - t^n)$$

provided that the arbitrary constant λ satisfies the inequality

$$\lambda > \max[a/2]$$

and the boundary conditions are also collocated at $t^{n+1/2}$.

Since Equation 15 is an elliptic equation, it can be solved by either the GVM or GEM.

NUMERICAL EXAMPLES

As an elementary example of the application of the GVM to parabolic problems, consider the very simple ground-water flow equation

$$SD_t u = T \nabla^2 u + Q(\underline{x} - \underline{x}_0)$$

defined over a homogeneous domain of 2 600 by 2 000 m, with S the storage coefficient (= 10^{-3}), u the hydraulic head, T the transmissivity (= 100 m^2) and Q (= - 1 000 m³/d) the rate at which water is extracted from the single sink situated at the point \underline{x}_0 = (1 300, 1 000). For initial and boundary conditions given by

$$u(x,y,0) = 0$$
 and $u(x,y,t) = 0$ on the boundary,

this problem has the analytical solution [Bear (1979)]

$$u(r, \theta, t) = [Q/(4 \pi T)] \int_{z}^{\infty} [\exp(-v)/v] dv$$
 17
where $z = Sr^2/4Tt$.

Equation 16 contains a logaritmic singularity at the sink which influence the solution adversely [Bakkes and Botha (1980)]. They circumvented this difficulty in the FEM solution of the same problem by subtracting the singularity, using a Green's function approach. This same procedure can also be applied in

the global variational and global element methods [Bakkes (1984)].

To investigate the behaviour of the GVM, Equation 16 was solved with the GVM, using a 5 x 5 Chebyshev polynomial approximation and the errors computed from Equation 17. The results are compared with that obtained by Bakkes and Botha (1980) for the finite element solution in Figure 2. The accuracy of the solution is clearly remarkable, particularly if it is kept in mind that the finite element solution was also corrected for the singularity and calculated, using a mesh consisting of 85 quadratic elements (292 nodes).

The final example to be considered here is that of an aquifer, the plan view of which is given in Figure 3. The aquifer is bounded by a series of leaky dykes. The domain of the aquifer can be naturally divided into two subdomains. In element 1 the average transmissivity is $2\,000\,\mathrm{m}^2$ and in element $2\,1\,000\,\mathrm{m}^2$. The storage coefficient is $2\,x\,10^{-2}$ across the aquifer. There are 19 wells present in the aquifer of which nine are used as production wells and the rest for observation. The pumping rates in the nine production wells are constant.

In order to apply the GEM to this irregular domain, transfinite interpolation had to be used. The efficiency of this form of map to transform an irregular domain onto a square one, can be judged from the blended function map of the aquifer given in Figure 4.

The behaviour of the aquifer was simulated, using the GEM with an 8 x 8 Chebyshev approximation on each element. Singularities caused by the production wells was subtracted using the procedure described above. In the case of the finite element simulation, the mesh shown in Figure 5 was used with linear basis functions. The simulation was conducted for the period June 1981 to August 1982.

The observed and computed heads are compared numerically in Table 1 and graphically in Figure 6. Although the drawdowns simulated by the GEM differs from those actually observed, the same applies to the FEM simulation. In fact, the close agreement between the values obtained in both simulations suggests rather that the model was not accurately calibrated. It would thus not be wrong to conclude that the GEM can be used with the same success as the FEM in simulating an actual aquifer.

TABLE 1. Observed and simulated hydraulic heads at the observation wells as for August 1982

Well number	Observed head	GEM	FEM
1	1448,3	1451,6	1450,7
4	1451,3	1450,6	1449,8
5	1454,0	1454,8	1454,2
6	1453,4	1453,9	1453,3
7	1465,0	1461,2	1461,0

CONCLUSION

In conclusion, it can be said that the GEM has some definite properties to recommend it as a method for simulating ground-water flow and related phenomena. The most outstanding of these are perhaps the ease with which the convergence of the method can be studied and singularities handled. This does not imply that the GEM is better than the FEM. In fact, it is doubtful whether the GEM can compete with the FEM in situations where the aquifer is highly inhomogeneous. Nevertheless, as indicated by the present study, there are problems where it may be preferred above the FEM.

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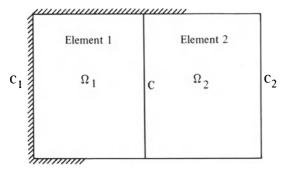


Figure 1. An example of two global elements.

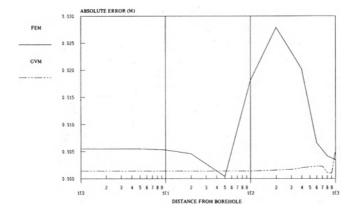


Figure 2. Maximum absolute errors observed in the GEM and FEM solutions of Equation 16.

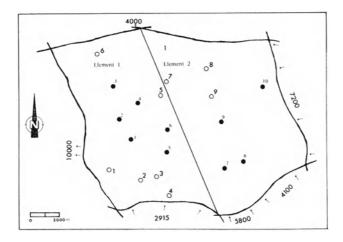


Figure 3. Plan view of aquifer used in present simulation.

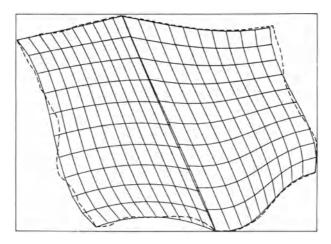


Figure 4. Blending function map of aquifer in Figure 3.

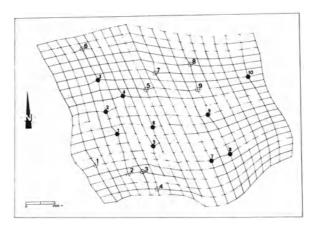


Figure 5. Finite element mesh used in simulating the aquifer in Figure 3.

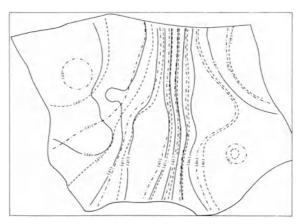


Figure 6. Observed and computed heads in the aquifer (August 1982). (——observed, - · - · GEM, - - - FEM).

SUMMARY

The main objective of the present paper is a study of variational and related methods defined over global regions. It is shown how a variational functional can be constructed for elliptic problems which allows basis functions that do not satisfy any boundary conditions. This functional is then extended to include problems where the domain is divided into a number of subdomains and parabolic problems. A comparison with the finite element method indicates that the method is useful, particularly in those cases where the domain can be divided into a small number of global elements.