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Assessing the Accuracy of a Finite Element Code in Solving the Advection–Diffusion Equation Using the Gauss Pulse Test

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Abstract

Using the Galerkin Finite Element Technique, a numerical code to study groundwater systems is being developed. This code has been applied to the Gauss Pulse Test to determine the accuracy of a number of solution schemes: in particular, which value of theta in the numerical time step theta algorithm gives the most accurate solution of the two-dimensional advection–diffusion equation. The theta algorithm enables time stepping to be performed explicitly $(\theta = 0)$, implicitly $(\theta = 1)$ and any combination thereof $(0 < \theta < 1)$.

Whilst the Gauss pulse test is a benchmark problem for assessing advection–diffusion type equations, it has predominantly been used to assess finite difference methods. Here however, it is used to evaluate a finite element scheme. A brief overview of the code is given, and various results for the Gauss pulse test discussed.

Introduction

Water is one of the most important resources to the continuing development of South Australia: in particular, groundwater, which is often the only source for drinking and/or irrigation water. To manage this resource properly, and prevent both the onset and spread of dryland salinity due to rising groundwater levels, it is important to be able to accurately predict how the system behaves.

In part this can be achieved through the use of numerical models which can simulate the system and how it responds to groundwater withdrawal, surface water injection and changes in recharge. It is then possible to simulate the system under the conditions of proposed management plans, enabling the effectiveness of each plan to be ascertained.

It is of paramount importance that any numerical code to be used in the study of a physical system be first shown to accurately solve those equations governing the system of interest. The system to be simulated using the code discussed in this paper is the groundwater aquifer beneath Padthaway in the South East of South Australia. A rising groundwater table and subsequent increasing levels of salinity have created the need for a management tool capable of determining the effects of current and future groundwater practices on the groundwater system. In terms of numerically modelling the movement of salt within the aquifer, this requires the accurate solution of an advection–diffusion type equation.

Whilst there are a number of commercial and public domain codes available for solving such an equation, the code developed by the authors is also suitable for solving the two–dimensional, density–dependent groundwater flow and solute transport equations, for which there are very few codes [8]. Furthermore, of these few suitable codes, the user generally does not have the ability to access the source codes to evaluate the solution techniques applied within the code.

The aim here is to determine the most accurate and most appropriate solution technique available within an especially developed numerical code so that upon application to the Padthaway groundwater system, the accuracy of simulation results is more assured.

The Numerical Code: SATFAT

Using the Galerkin Finite Element Technique, a numerical code to solve the flow and solute transport equations for fluids in porous media has been developed. The code is called SATFAT; an acronym for SATurated Flow And Transport. It has a number of solution options including mass lumping, and direct and iterative matrix inversion, and uses the theta algorithm [1] for the discretisation of time. Having the ability to control the solution process allows the user to determine the effect of the solution technique on results. Thus, it is possible to objectively evaluate various solution options.

Direct matrix inversion is achieved using the sparse–matrix inversion routine GELB [2], and the Gauss–Seidel method used for iterative inversion. The latter is of several orders of magnitude faster than the former in most cases. Mass lumping is the technique of lumping mass at the nodes of an element so that the time derivative applied over the element is only discretised at each node. This process is of significant benefit in that it diagonalizes the global mass matrix making it more robust to invert. Zienkiewicz and Taylor [11] present a number of procedures to achieve this.

SATFAT is being developed to solve constant and variable density versions of the governing equations for fluid flow and solute transport through porous media. To model the Gauss pulse test [6] it is necessary to only solve the constant density solute transport equation, which in this case can be simplified to the advection–diffusion equation

$$\frac{\partial \omega}{\partial t} + u\frac{\partial \omega}{\partial x} + v\frac{\partial \omega}{\partial y} - \alpha_x \frac{\partial^2 \omega}{\partial x^2} - \alpha_y \frac{\partial^2 \omega}{\partial y^2} = 0, \qquad (1)$$

where ω is the solute mass fraction, u and v are the velocities [m/s], and α_x and α_y [m^2/s] the diffusivities in the x- and y-directions respectively.

Applying the method of weighted residuals to equation (1), and using the Galerkin technique with bi–linear quadrilateral elements yields the following elemental expression

$$A\omega + B\frac{\partial \omega}{\partial t} = 0, \qquad (2)$$

with A and B representing coefficient matrices that are obtained from integrating the appropriate element arrays. Derivations of these matrices can be found in Narasimhan [3] and Pinder and Gray [7]. A finite difference approximation is used to discretise time which after application of the theta algorithm yields:

$$\omega^{n+1} = (B/\Delta t + A\theta)^{-1}((B/\Delta t - A(1-\theta))\omega^n), \qquad (3)$$

where $\theta = 0, 0.5, 1$ correspond to the explicit, Crank–Nicolson implicit (CNI) and implicit methods respectively. It has been shown by Giraldo and Neta [1] that such schemes are conditionally stable for values of theta in the range $(0 \le \theta < 0.5)$, and unconditionally stable for $(0.5 \le \theta \le 1)$. Here the aim is to assess accuracy as a function of θ.

To determine how accurately SATFAT solves the advection–diffusion equation, it has been applied to the Gauss pulse test.

The Gauss Pulse Test

The Gauss pulse test has been extensively used to assess the accuracy of finite difference schemes in solving the advection–diffusion equations in one dimension [4, 10] and two dimensions [5, 6]. Truscott and Turner [9] applied the Gauss pulse test to a control volume finite element method with moderate success. For the two-dimensional case, the advection-diffusion equation (1) with constant u, v, α_x and α_y is solved in the rectangular region $0 < x < X$, $0 < y < Y$, for $0 < t < T$.

The exact solution to this problem is given by Noye [6] to be

$$\omega(x,y,t) = \frac{1}{\tau}\exp\left(-\frac{\phi(x,t)}{\alpha_x\tau} - \frac{\psi(y,t)}{\alpha_y\tau}\right), \qquad (4)$$

where $\tau = 4t+1$, $\phi(x,t) = (x-ut-x_c)^2$, $\psi(y,t) = (y-vt-y_c)^2$, for the case with initial condition $\omega(x,y,0)$, and boundary conditions $\omega(0,y,t), \omega(X,y,t), \omega(x,Y,t)$ and $\omega(x,0,t)$. Physically, the initial condition describes a two-dimensional Gauss pulse of height 1m centred at $(x_c, y_c) = (0.5\text{m}, 0.5\text{m})$.

The 2D projections of the initial pulse and the resultant pulse after $t = 1.25$ seconds are shown in figure 1.

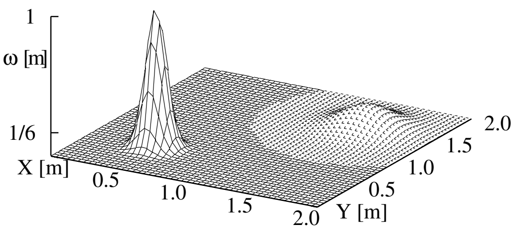

Figure 1: 2D projections of the initial (left) and resultant (right) pulses after $t = 1.25s$.

The coefficients of the diffusion terms are chosen to be $\alpha_x = \alpha_y = 0.01$ m^2/s and the flow is uniform in both the x- and y-directions at $u = v = 0.8$ m/s. After a period of $t = 1.25$ seconds the pulse has travelled to a position centred at $(x,y) = (1.5\text{m}, 1.5\text{m})$ and has reduced in height to 1/6m. The reduction in peak solute concentration is due to diffusion whilst the change in location of the peak is due to advection.

Application of SATFAT to the Gauss Pulse Test

The Gauss pulse was simulated using the constant density solute transport option within SATFAT. For the purpose of comparison, the solution domain was restricted to $X = Y = 2$m with a grid spacing of 0.025m in both the x- and y-directions. This corresponded to a square grid of 80 x 80 elements with bi–linear interpolation functions. A total of 125 time steps of equal duration of 0.01 seconds were used to give a simulation time of $t = 1.25$ seconds. Solution options examined were matrix inversion, mass lumping and the value of theta.

Table 1 gives the various options used for each solution scheme, and the height of the Gauss pulse after $t = 1.25$ seconds.

Ref.	Inversion	Mass Lumping	θ	Peak
G1	direct	no	0.00	0.192m
G3	direct	yes	0.00	0.193m
G4	iterative	yes	0.00	0.193m
G5	direct	no	0.25	0.177m
G7	direct	yes	0.25	0.178m
G8	iterative	yes	0.25	0.178m
G9	direct	no	0.50	0.166m
G11	direct	yes	0.50	0.167m
G12	iterative	yes	0.50	0.167m
G13	direct	no	0.75	0.148m
G14	iterative	no	0.75	0.148m
G15	direct	yes	0.75	0.149m
G16	iterative	yes	0.75	0.149m
G17	direct	no	1.00	0.134m
G19	direct	yes	1.00	0.136m

Table 1: Solution options and Gauss pulse peak height for each of the solution schemes. The exact solution gives a pulse of height 1/6m.

Note that G2, G6, G10, G18 and G20 have been omitted as in each case the matrix to be inverted wasn't diagonally dominant so iterative inversion wasn't used.

Gauss Pulse Test Results

Cross-sections of pulse height through the y=1.5m transect are shown in figures 2, 3, 4 and 5. The cross-sections are grouped according to the solution options of matrix inversion and mass lumping. For each group it is then simple to identify which value of theta (0, 0.25, 0.50, 0.75 or 1.00) gives the most accurate solution. Contour plots of resultant pulse height (solute concentration) for a selection of the solution schemes are shown in figure 6.

For all schemes, the location of the peak after $t = 1.25$ seconds was either at (1.5m,1.5m) or within 0.025m of this. Any numerical dispersion introduced by the code is evident in the uneven diffusion of the Gauss pulse, and can be observed in figure 6(b), (c), (e) and (f). Numerical dispersion refers to the apparent dispersion of the solute due to numerical error in approximating the exact equation (1) with difference equations. In finite differences, it has been shown to be a function of time step size and velocity [6], and can be minimised by balancing the magnitude of the time step with the velocity of the flow.

After running all schemes using 125 time steps of 0.01 seconds, it was found that to attain a stable solution for the explicit and near explicit schemes G1-8, it was necessary to increase the number of time steps to 250, with the requisite decrease in the magnitude of the time step. By comparing the time taken for each solution scheme, the expectation that the iterative schemes were considerably faster than the direct inversion was confirmed as overall, the direct inversion schemes took some twenty times longer than the iterative schemes.

For a given value of theta and choice of mass lumping, the results for the Gauss pulse test using iterative inversion were comparable with those using direct inversion. This is shown in table 1 when comparing G3 with G4, G7 with G8, G11 with G12, and so on. The small differences observed can be eliminated by simply increasing the number of iterations for the iterative inversion routine at each time step.

As shown in figure 2 and table 1, the ranking of accuracy of the non-mass lumped, direct inversion schemes in terms of peak height is G9,G5,G13,G1,G17.

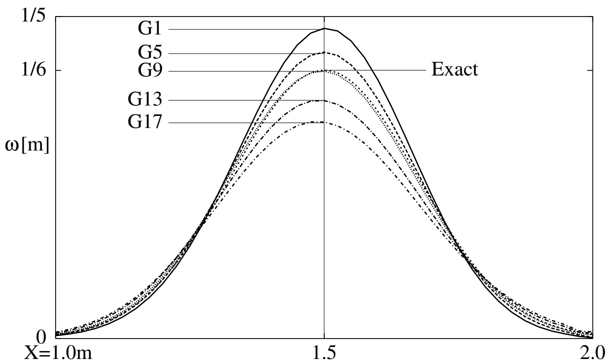

Figure 2: Cross-sections for schemes using exact inversion and no mass lumping (G1,G5,G9,G13,G17) compared with the exact solution.

Of these the most accurate is the CNI scheme ($\theta = 0.5$). This scheme also exhibits the least dispersion, with the fully implicit and explicit schemes G17 and G1 exhibiting the most dispersion.

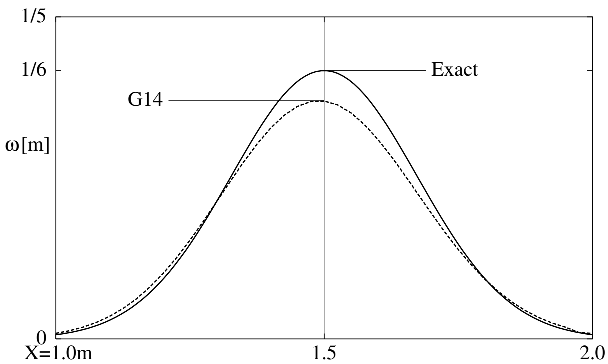

Figure 3: Cross-section for the non-mass lumped scheme using iterative inversion (G14) compared with the exact solution.

The only non-mass lumped scheme that could utilise iterative inversion was the near implicit scheme G14. This produced a peak height of 0.148m; its contour plot was very similar to that of scheme G13 shown in figure 6(e) indicating numerical dispersion. As discussed above, G14 was the only case where the coefficient matrix was diagonally dominant, indicating that although mass lumping is numerically questionable it does lead to a more robust and invertible matrix [11].

Of the mass lumped schemes using direct inversion, the CNI scheme G11 was the most accurate. The ranking of accuracy of these schemes was G11,G7,G15,G3,G19. There was very little difference between the non-mass lumped and mass lumped schemes using direct inversion for a given value of theta, other than a small increase in the height of the Gauss pulse for the mass lumped schemes. The numerical dispersion exhibited in each of these schemes was comparable to that exhibited in the equivalent non-mass lumped schemes.

Results for the Gauss pulse test with $\theta = 0.5$ from SATFAT are more accurate than those developed by Truscott and Turner [9] using a control volume finite element method, and compare favourably to those published by Noye [6] using high–order fully implicit finite difference schemes. Additional results for the Gauss pulse test using alternative values for the velocities u and v, and diffusion terms α_x and α_y have yielded a similar pattern of accuracy in terms of θ and choice of inversion routine.

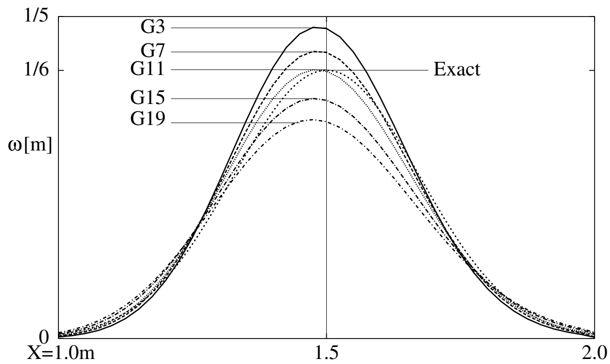

Figure 4: Cross-sections for schemes using exact inversion and mass lumping (G3,G7,G11,G15,G19) compared with the exact solution.

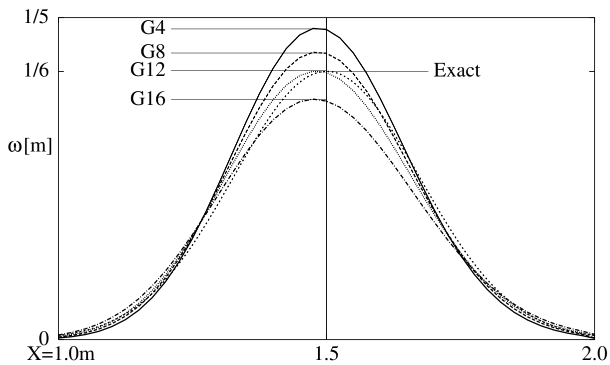

Figure 5: Cross-sections for schemes using iterative inversion and mass lumping (G4,G8,G12,G16) compared with the exact solution.

Conclusion

The most accurate results in terms of both the height and location of the Gauss pulse peak were found to be those using the CNI ($\theta = 0.5$) schemes. This was irrespective of choice of matrix inversion or mass lumping. The CNI schemes also exhibited the least numerical dispersion, with the non-mass lumped scheme the best.

Whilst there is only a small difference in results between schemes using direct and iterative inversion, the substantial but not unexpected increase in computational time for direct inversion schemes over those using iterative inversion, makes the latter a more suitable choice where iterative inversion can be used. For the CNI scheme this implies the need for mass lumping to ensure the mass matrix is diagonally dominant.

This analysis has shown that using techniques other than the CNI scheme produces errors up to approximately 20% because of numerical dispersion. This can have significant implications in terms of assessing management alternatives for the Padthaway groundwater system, and any other areas to which this or similar codes are applied. In practice, the choice of values for such parameters as α_x and α_y can have dramatic effects upon modelling results. However, having the ability to accurately solve the governing equations enables the modeller to apply a range of inverse techniques in helping choose parameter values, which ultimately allows for a more useful management tool.

In conclusion, model results of the Gauss pulse test show the most accurate solution scheme to be the non-mass lumped, CNI scheme.

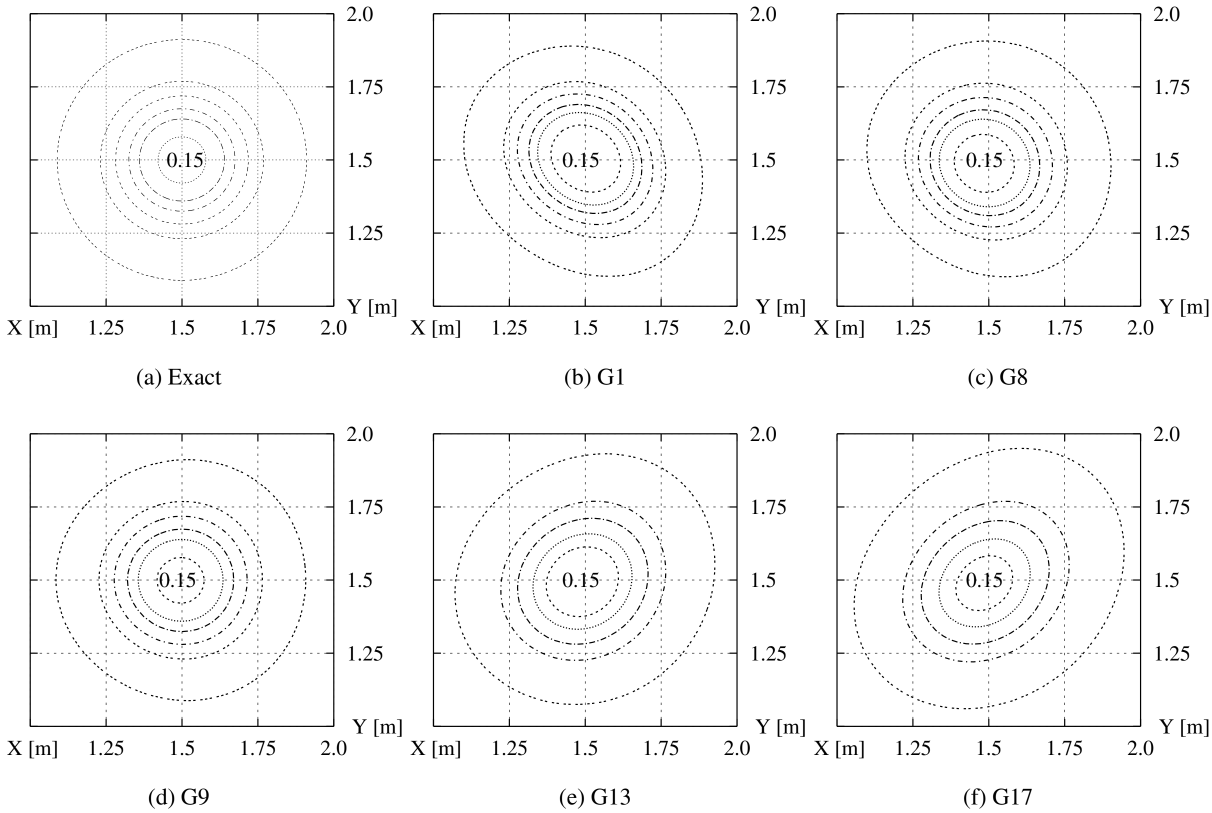

Figure 6: Contour plots of the exact solution and the solution schemes G1,8,9,13,17 showing isolines of 0.15 (where applicable), 0.12, 0.10, 0.075, 0.05 and 0.01m in order of increasing radius.

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