Locally refined block-centred finite-difference groundwater models: evaluation of parameter sensitivity and the consequences for inverse modelling

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Abstract Models with local grid refinement, as often required in groundwater models, pose special problems for model calibration. This work investigates the calculation of sensitivities and the performance of regression methods using two existing and one new method of grid refinement. The existing local grid refinement methods considered are: (a) a variably spaced grid in which the grid spacing becomes smaller near the area of interest and larger where such detail is not needed, and (b) telescopic mesh refinement (TMR), which uses the hydraulic heads or fluxes of a regional model to provide the boundary conditions for a locally refined model. The new method has a feedback between the regional and local grids using shared nodes, and thereby, unlike the TMR methods, balances heads and fluxes at the interfacing boundary. Results for sensitivities are compared for the three methods and the effect of the accuracy of sensitivity calculations are evaluated by comparing inverse modelling results. For the cases tested, results indicate that the inaccuracies of the sensitivities calculated using the TMR approach can cause the inverse model to converge to an incorrect solution.

Key words local grid refinement; MODFLOW; telescopic mesh refinement; UCODE

INTRODUCTION

Many groundwater modelling studies require or would benefit from a finer grid in a specific part of the domain to represent localized phenomena with greater resolution. Examples include regions of contamination where solute transport simulations are of interest; regions of rapidly varying hydraulic gradients, such as near pumping or injection wells; and regions bordering surface-water bodies where both chemical processes and detailed representation of gradients may be important. Within the commonly used finite-difference framework used in MODFLOW and other groundwater models, there are several methods that modellers can use to locally refine the grid. Although these methods all solve the same partial-differential equation, there are differences due to the nature of the discretization procedure. Mehl & Hill (2002a) have shown that some local grid refinement methods for finite-difference grids can have significant discrepancies along the interfacing boundary between the coarse and refined grids, which can cause inaccuracies in the forward solution. An important question is how the differences in the discretization affect model calibration. This can be quantified using formal inverse modelling. This work addresses this question by comparing perturbation-calculated sensitivities and inverse modelling results for three choices of local grid refinement within a finite-difference framework.
The first local grid refinement method evaluated is a variably spaced grid. This is a common approach that can work very well. Its drawbacks are related to the need to extend the mesh lines out to the boundary of the domain. This can result in refinement in areas where such detail is not needed. Also cells with a large aspect ratio are generally produced near the periphery of the domain, which can cause numerical errors (de Marsily, 1986, p.351). Finally, variably spaced grids are less flexible than the methods discussed below in terms of designing the grid and data input.

The second local grid refinement method is commonly used in groundwater modelling studies and is known as telescopic mesh refinement or TMR (for example, Ward et al., 1987; Leake & Claar, 1999; Davison & Lerner, 2000). This approach uses the results of a coarse-grid regional model simulation to provide head or flux boundary conditions for a refined-grid local model. This approach is very flexible and relatively easy to implement. However, the coupling of heads or fluxes between the models occurs in one direction—from the coarse grid to the refined grid—and there is no mechanism to provide information back to the coarse grid. Typically, after running both models, there may be a significant discrepancy in either heads or fluxes, whichever is not used in the coupling of the two models. Furthermore, there is no standard procedure for adjusting the models such that they will have better agreement, leaving the modeller unsure of whether the agreement between the models is adequate or not.

The third local grid refinement method, developed by the authors, is an iteratively coupled method with shared nodes (Szekely, 1998; Mehl & Hill, 2002a,b), which incorporates a feedback from the refined grid to the coarse grid, ensuring that heads and fluxes are consistent between the grids. This method is similar to directly coupled methods in which the matrix equations are modified to account for the irregular connections along the interface between the two grids (Haefner & Boy, 2001; Schaars & Kamps, 2001), except that the coupling has been formulated with shared nodes and is performed iteratively instead of directly. The drawback of directly coupled methods is that the irregular connections can cause the matrix to be asymmetric and lose diagonal dominance (Edwards, 1996), thus hindering convergence. In contrast, the iterative approach considered here places the irregular components of the matrix on the right-hand side of the matrix equations, updating the right-hand side with each iteration. This has the advantage of maintaining a conventional matrix stencil for each solution so that efficient solvers based on this stencil can be used without modification.

The iteratively coupled method with shared nodes has the advantage of being as flexible as the TMR methods. Its drawback relative to the variably spaced and TMR methods, to which it will be compared, is that it is less accurate than the former and requires more CPU time than the latter. Accuracy and execution time issues have been investigated by Mehl & Hill (2002b); this work focuses on how the different levels of accuracy achieved by variably spaced grids, TMR, and the iteratively coupled method with shared nodes, affects the calculated sensitivities and regression performance.

**METHODS**

A synthetic test case based on a sand tank experiment (Garcia, 1995) was used to simulate flow through a two-dimensional (2-D) porous medium, and is shown in Fig. 1. Results are compared to a fine-grid discretization, which provides the reference
simulation. The fine grid has 450 rows and 972 columns, with cell dimensions of 1.028 m and 1.0 m in the horizontal and vertical directions, respectively. For the local grid refinement methods, the embedded grid has 100 rows and 154 columns with cell dimensions equal to the fine grid. The area of the locally refined model is shown enclosed in a dashed rectangular line in Fig. 1, which includes a pumping well that extracts 5.5 m$^3$/s. The coarser outer grid has 50 rows and 108 columns, with cell dimensions of 9.25 and 9.0 m in the horizontal and vertical directions, respectively. The ratio of refinement is 9:1 (nine local cells span the width of one coarse grid cell). The variably spaced grid has 275 rows and 380 columns. The coarsest mesh spacing is never greater than the coarser outer grid, and the finest mesh spacing is equivalent to the embedded refined grid.

All simulations were conducted using MODFLOW-2000 (Harbaugh et al., 2000). The TMR method was implemented using MODTMR (Leake & Claar, 1999), which can couple the models using heads or fluxes. Both options were investigated.

The effects of the different discretization schemes are evaluated by comparing sensitivity and inverse modelling results. Sensitivities are calculated for 96 head observations and are generated with UCODE (Poeter & Hill, 1998) using central differences and perturbations of 5%. Other perturbation values were tested and it was found that a value of 5% produced the closest match to MODFLOW-2000’s analytically calculated sensitivities (Hill et al., 2000). Of the 96 observations, 61 are located within the area of local refinement, and 35 are outside of this region. Inverse modelling was also performed with UCODE, using the same 96 observations to estimate the five values of transmissivity shown in Fig. 1. The success of inverse modelling depends both on the accuracy of the sensitivities and the inverse algorithm used. The influence of forward-and central-difference sensitivities and three different search techniques are investigated.

**COMPARISON OF SENSITIVITIES**

Sensitivities to the 96 observations for each of the transmissivities were calculated using all the discretization methods. The root mean square of the percent errors relative to the fine grid (equation (1)) are shown in Table 1, and are calculated as:

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^{96} \left( \frac{s_i' - s_i}{s_i} \times 100 \right)^2}{96}}$$

(1)
Table 1 Comparison of root mean square percent sensitivity errors of the discretization methods for the transmissivities shown in Fig. 1.

<table>
<thead>
<tr>
<th>Discretization</th>
<th>T1 % Error</th>
<th>T2 % Error</th>
<th>T3 % Error</th>
<th>T4 % Error</th>
<th>T5 % Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Variably spaced</td>
<td>13.60</td>
<td>0.1288</td>
<td>0.9437</td>
<td>0.2550</td>
<td>0.1321</td>
</tr>
<tr>
<td>TMR-head</td>
<td>21.47</td>
<td>1.766</td>
<td>7.604</td>
<td>6.036</td>
<td>3.205</td>
</tr>
<tr>
<td>TMR-flux</td>
<td>16.24</td>
<td>2.066</td>
<td>60.22</td>
<td>105.2</td>
<td>5.577</td>
</tr>
<tr>
<td>Iteratively coupled</td>
<td>10.58</td>
<td>1.380</td>
<td>0.9457</td>
<td>1.630</td>
<td>2.921</td>
</tr>
</tbody>
</table>

\(^1\)Local model uses specified-head boundary conditions derived from the regional model.
\(^2\)Local model uses specified-flux boundary conditions derived from the regional model.

where RMSE is the root mean square error, \(s_i\) is the sensitivity for the \(i\)th observation calculated using the fine grid, and \(s_i'\) is the sensitivity for the \(i\)th observation calculated using one of the other discretization methods. These results demonstrate that the variably spaced grid has the least error, as expected, while the TMR methods with coupling using fluxes have the greatest error. The iteratively coupled method has errors that are always less than the TMR methods, which indicates that the feedback between both grids is important for accurate sensitivity calculations. Indeed, the added flexibility provided by the iteratively coupled method over the variably spaced method does not generally seem to be burdened with a large degree of inaccuracy in the sensitivities.

**EFFECT ON INVERSE MODELLING**

The errors in sensitivities can affect inverse modelling. This issue was addressed by using UCODE, with each of the discretization methods, to estimate the five values of transmissivity by nonlinear regression. The 96 head observations used were generated, without adding noise, using the fine-grid discretization and the parameter values shown in Fig. 1. The same set of starting parameter values, which were changed from the true values shown in Fig. 1, were used in the inverse simulations. The inverse modelling was evaluated based on how well the five transmissivities returned to their true values, thus lowering the sum of squared residuals. Sensitivities are often calculated using the more computationally frugal but less accurate forward-difference method (fwd), so this method was also considered. UCODE implements the modified Gauss-Newton (G-N) method to perform the regression, with the ability to include quasi-Newton (Q-N) updating. In addition, the double-dogleg (DOG) trust region approach (Dennis & Schabel, 1996) was added to UCODE so that the three options could be investigated.

For this test case, Fig. 2 shows how the sum of squared residuals is lowered as the regression proceeds and the total number of function evaluations at the final iteration, for each of the discretization methods. The more accurate central differencing (cen) is important for good convergence of the G-N method when using the variably spaced grid (Fig. 2(a)). These results also demonstrate that the Q-N updating and double-dogleg approach can substantially reduce the number of function evaluations needed for convergence, thus reducing CPU time. The inaccurate sensitivities calculated using
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Fig. 2 Regression results using the Gauss-Newton (G-N) and quasi-Newton (Q-N) methods with forward (fwd) and central (cen) differencing for simulations using: (a) a variably spaced grid, (b) a TMR coupled using heads, (c) a TMR coupled using fluxes, and (d) an iteratively coupled grid. The total number of function evaluations is indicated at the final iteration.

the TMR methods (Fig. 2(b) and (c)) hindered convergence of the G-N method, and even the more accurate central differencing was unable to alleviate this problem. For these cases, the resulting parameter estimates were grossly different from the true parameter values. However, in the case of coupling with heads, good convergence was achieved using either Q-N updating or the double-dogleg strategy. In contrast, the sensitivities calculated using the iteratively coupled method were accurate enough that good convergence was achieved for all scenarios (Fig. 2(d)).

CONCLUSIONS

This work demonstrates that different methods of local grid refinement can have a substantial effect on parameter sensitivity calculations, which in turn can affect inverse modelling results. For the case presented, the variably spaced grid method of local grid refinement is most accurate in terms of sensitivity calculations, while the TMR methods were least accurate. The iteratively coupled method was always more accurate than the TMR methods and approached the accuracy of the variably spaced grid. The results also show that the accuracy of the sensitivity calculations influence the regression, and some of the inaccuracy can be overcome by using more
sophisticated search techniques, as shown by the quasi-Newton and double-dogleg results. However, for the TMR method coupled using fluxes, the sensitivities were too inaccurate to produce good convergence results, even when using quasi-Newton updating. In contrast, the iterative local grid refinement method with shared nodes developed by the authors performed well both with the most rudimentary search technique (G-N) and least accurate sensitivities considered (forward differencing).

REFERENCES


