New and Contrasting Approaches to Local Grid Refinement

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ABSTRACT

A common criticism of finite-difference groundwater simulators is the cumbersome approach to the refined simulation of local areas within a regional grid. If a modeler wishes to finely discretize a small area within a large grid, the many elongate cells that result from gradational refinement schemes are at best aesthetically displeasing, and at worst may compromise the simulation. We evaluate contrasting approaches to local grid refinement (LGR) adopted in recent releases of the USGS MODFLOW code and the ZOOMQ3D code – the latter a collaborative venture between Birmingham University, UK, the Environment Agency (EA), UK, and the British Geological Survey (BGS). An overview of the theory underpinning each method is followed by the application of each program to simulate a standard benchmark problem. Each program is then used to simulate a synthetic test case. The synthetic test case is based upon a real-world site in which high-capacity pumping centers dominate the groundwater flow system within the focus area. In each instance simulations are also conducted using MODFLOW with standard gradational refinement for comparison. Discussion of the results focuses on ease of development; simulation stability; and accuracy in representing heads in the refined area. Some mention is made of computational effort. A brief summary is provided of capabilities of each method that extend beyond those tested here. This evaluation was not conducted in a rigorous manner that could support such a quantitative comparison of methods, and was not intended as such. The principal purpose of this evaluation is to expose modelers to the refinement options that are available.

INTRODUCTION

Numerical groundwater flow models are constructed where assumptions underlying analytical methods are violated to an unacceptable degree. Solution of the groundwater flow partial-differential equation is typically accomplished through finite differences or finite elements. In each, the domain is discretized into cells or elements and a flow equation is constructed for each (active) cell or element. The collective equations are solved, together with boundary condition constraints, to provide a head solution. Wang and Andersen (1982) outline the finite difference and finite element techniques. Implementation of block-centered finite-differences in MODFLOW is described by McDonald and Harbaugh (1988). Although Harbaugh (1992) showed that generalized finite differences may under some circumstances be extended to include curvilinear cells and cells of more complex geometries, common implementations of the finite-difference method are restricted to regular rectilinear cells. Common simulators constructed within this framework suffer the criticism that the gradational refinement required to simulated detail in a small area leads to many elongate cells through the domain, with fairly well known consequences. Proponents of the finite-element technique, which is not hampered by this problem to such a degree, highlight this as a significant downfall of the finite-difference method. This paper reviews and contrasts some approaches to LGR that are available to finite-difference practitioners. The evaluation is not comprehensive, and readers are recommended to review the references provided for further, detailed, information. LGR methods evaluated in this paper are first described, and then applied to a steady-state and transient synthetic problem, based upon a real-world model. Some alternative methods that are not evaluated in this paper are also alluded to for completeness.

OVERVIEW OF REFINEMENT METHODS

Gradational Mesh Refinement (GMR)

GMR involves the gradational refinement of cell sizes from a “background” of large cells to a local area of small cells, often referred to as a “submodel.” This is the most commonly adopted refinement approach, and that which is most commonly criticized. The principal disadvantage of this approach is the large number of cells that are produced, many with large aspect ratios, and the numerical instabilities that can result. Advantages of this approach include a regular structure between adjacent cells; a single model that is solved in a single (iterative) matrix equation; and hence “real-time” feedback between the coarse and fine grid areas through this single matrix solution. In this document this approach, as implemented within the MODFLOW programs, is referred to as “MF-GMR,” and is illustrated in Figure 1a for the synthetic test case. GMR is the *de facto* benchmark for evaluations presented here.

Local Grid Refinement (LGR)

LGR links two or more different-sized grids – that is, a coarse (parent) grid covering a large area and incorporating regional boundary conditions, and one or more fine (child) grids covering the local area(s). The link between the parent and child grids can be accomplished as a one-way coupling, where conditions simulated by the parent are imposed on the child boundaries; or in a way that includes communication and hence two-way feedback between the parent and child. Couplings with feedback can be accomplished through (a) the use of separate models that are iteratively solved until global convergence is achieved; or (b) by modifying the finite difference equations to solve the redefined problem as a single matrix equation (de Marsily, 1986). The two contrasting approaches that are next described each embody one of these methods. Disadvantages of this approach include an inconsistent structure across the parent-child boundary; and, in the separate-model method, the development and maintenance of separate model files. Advantages of this approach include the regular structure within the child; the large reduction in the total number of cells required to simulate the problem; and, on many occasions, the reduced computational burden versus GMR methods.

a. Iterative Solution Approach

Mehl and Hill (2002, 2004, 2005) describe an iterative LGR method that couples parent and child models using shared nodes. That is, parent and child grids are constructed so that select nodes of the parent coincide with boundary nodes of the child. The iterative solution adjusts heads and fluxes of both grids to achieve convergence. A single iteration requires one parent-model solution and one child-model solution, so that execution time per iteration equates to approximately the sum of the individual models. The number of iterations required is problem specific. The approach introduces some error into the solution, but Mehl and Hill (2004) demonstrate that this is less than in one-way couplings. This approach is incorporated in the most recent version of MODFLOW, MODFLOW-2005, and is referred to here as “MF-LGR.” MF-LGR supports horizontal and vertical refinement (Table 1). An example grid geometry is illustrated in Figure 1b for the test case described here. In the current release only one block-shaped volume of local refinement can be simulated, though this is not a restriction of the method; and the shared-node coupling requires child-grid spacing that is an odd integer factor of the parent grid, for example, 1:1, 3:1, 5:1, 7:1.

b. Single Matrix Solution Approach

Jackson and Spink (2004) describe a quasi-3D groundwater simulator, ZOOMQ3D, that implements the single-matrix equation approach to LGR analogous to the method described by von Rosenberg (1982), and referred to throughout this study as “ZOOMQ3D.” As the name suggests the LGR capabilities of ZOOMQ3D are an important feature of the program. ZOOMQ3D constructs a modified form of the finite-difference equations that enables the solution of LGR problems within a single matrix equation. This enables ZOOMQ3D to support multiple child grids within a single parent; both even and odd refinements; and the definition of irregular child grids – that is, the child grid does not have to be a regular four-sided polygon. In the current release of ZOOMQ3D the maximum refinement factor is 1:5 of the parent grid, and vertical grid refinement is not supported (Table 1). An example grid geometry is illustrated in Figure 1c for the test case described here. The ZOOMQ3D code has been verified against a number of analytical solutions, and ZOOMQ3D simulations of steady-state and transient problems distributed together with USGS versions of MODFLOW are essentially identical. As part of this study we evaluated ZOOMQ3D simulations of several standard MODFLOW test cases and confirmed this. Note that while MODFLOW is block-centered, ZOOMQ3D is node centered, and this must be considered when comparing simulation results between the two programs.

Other Methods

Two methods that are not evaluated here – that is, Telescopic Mesh Refinement (TMR) and the Analytic Element Method (AEM) – are now briefly described. TMR typically involves gradational refinement much like GMR, however with the development of one or more *separate* child models. Child boundary conditions are defined by interpolation of heads, fluxes, or both from the parent (Leake and Claar, 1999). The coupling is one way, hence the modeler must develop methods to assess and redress the consistency of results along the boundary interface. If this is not undertaken errors may go undetected (Mehl and Hill, 2002). Since TMR is established and widely used it is not discussed further. The AEM can be used to define fluxes and heads as boundary conditions for one or more child models (Haitjema, 1995; Hnt, 2006). At least one of the authors has experience using the AEM for this purpose. However, though conceptually simple AEM applications are not widespread, perhaps due to lack of experience in the community and(or) the relative absence of training that could highlight the method's benefits.

SYNTHETIC APPLICATION

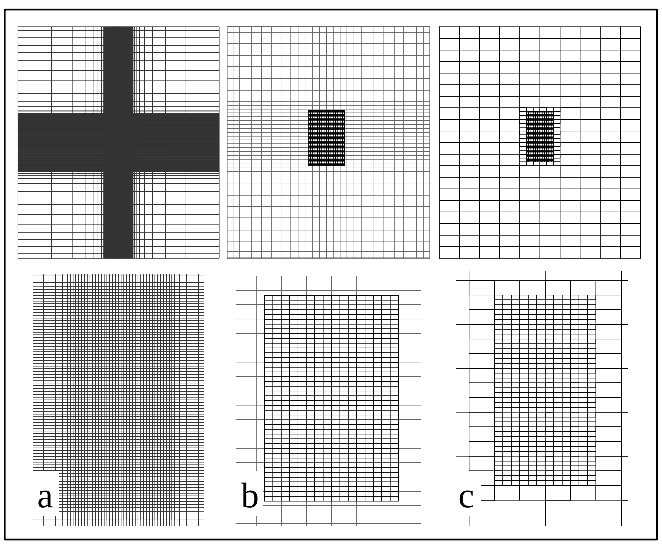

Figure 1. Regional and local grids used in evaluations.

The synthetic study is based on a comparison of steady-state and transient heads and drawdowns simulated in response to pumping at two closely-spaced wells within a single area of refinement embedded within a 6-layer model. The model structure is a simplification of a real-world application originally constructed in MODFLOW-2000 to evaluate the potential performance of a groundwater recovery (pump-and-treat) system. The principal simplifications are horizontal anisotropy and homogeneity; in addition, no head-dependent boundary conditions traverse the parent-child interface. The finite-difference grids used for each of the refinement methods are shown in Figure 1a (GMR. 40,000 nodes), Figure 1b (MF-LGR. 5,000 nodes) and Figure 1c (ZOOMQ3D. 4,600 nodes) respectively. The groundwater recovery wells are located in layers 5 (bottom left) and 2 (top right). The steady-state model includes no head-dependent boundary types. Steady-state heads in Layer 2 simulated by the three methods are superimposed on Figure 2. The transient model includes a river within the course (parent) grid and three observation wells designed to monitoring transient heads in response to pumping from the two recovery wells (Figure 3). The transient heads are illustrated in Figure 4. These illustrations of steady-state and transient heads suggest that – for the simple case described here - the two LGR methods produce comparable results to the more typical gradational refinement approach, but require a considerably smaller number of model cells - approximately one tenth for this simple problem. Simulation times for the steady-state models were all very rapid and essentially comparable, though the LGR methods did execute more quickly. Since the execution times were very rapid, part of this difference may be due simply to file input-output and other practical factors, rather than the actual time required to solve the problem. For the transient simulations, both ZOOMQ3D and MF-LGR required slightly more time to execute than the GMR model with the same time-stepping. However, it must be noted that this comparison is purely qualitative – the number of nodes differ between models, the solver(s) differ, and solver options were not rigorously explored. Therefore, run-time implications for large and(or) complex transient models are uncertain and not concluded or further explored here.

RESULTS AND DISCUSSION

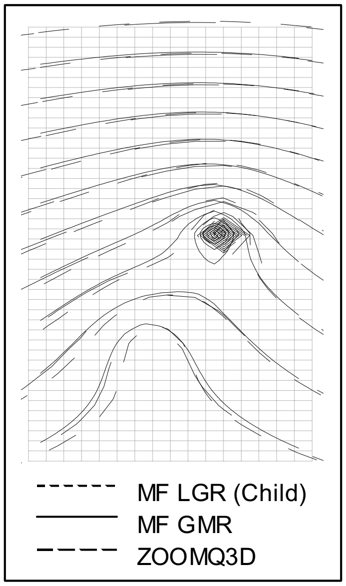

Figure 2. Steady-state simulation results.

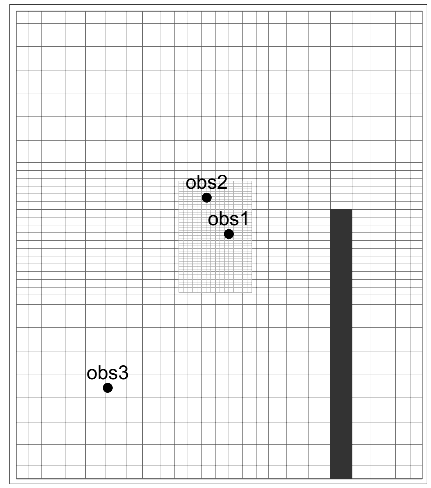

Figure 3. Transient model - observation wells and river.

This simple evaluation tested limited aspects of the simulation capabilities of MODFLOW-2005 local grid refinement code, referred to here as MF-LGR, and ZOOMQ3D. Table 1 gives a brief summary of certain capabilities of these programs together with other approaches not evaluated here. Clearly, local refinement approaches provide much of the improved accuracy and detail achievable by global refinement methods. In steady-state it is evident this is achieved with more rapid execution times. In the sole transient test simulations of both LGR methods were slightly longer than the GMR method, but a rigorous evaluation of solver options and convergence was not made. A current limitation of both the MF-LGR and ZOOMQ3D approaches is the inability to support advective-dispersive transport across the parent-child interface. This may limit the application of these methods for certain types of problems, such as groundwater remediation and contaminant fate analyses. Each method may encounter difficulties developing these capabilities using existing simulation programs due to the necessity of either (a) developing a complex mass-balance-constrained coupling or (b) modifying the standard finite difference transport equations. However, in terms of groundwater flow, modelers familiar with the MODFLOW programs will find that MF-LGR is easy to work with and offers immediate results. For modelers not accustomed with ZOOMQ3D a small investment of time is required to become familiar with the input file structure and the ZETUP pre-processor, but following this modelers will find the flexible zooming – and in particular, the multiple child capabilities - very accessible.

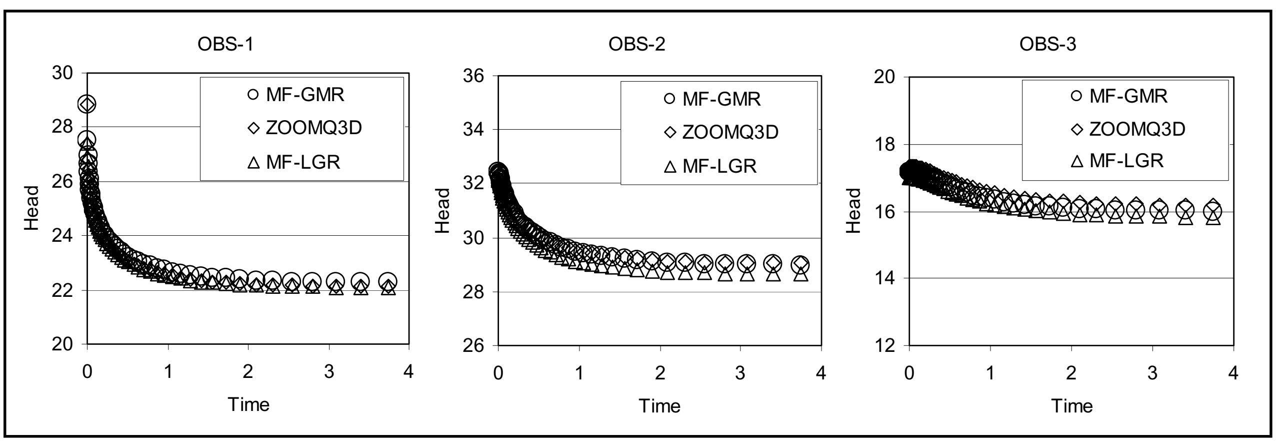

Figure 4. Hypothetical well hydrographs - Note: interpolation may lead to small differences.

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Scheme	Two-way Feedback	Multiple File Sets	Multiple Areas of Refinement	Vertical Refinement[1]	Hetero-geneity[2]	Particle Tracking[2]	Contaminant Transport[2]	Public Domain
MF GMR	Yes	No	Yes	No	Yes	Yes	Yes	Yes
MF TMR[3]	Manual?	Yes	Yes	No	Yes	No	No	Yes
MF LGR	Yes	Yes	Planned	Yes	Yes	(5)	(5)	Yes
ZOOMQ3D	Yes	No	Yes	Planned	Yes	Yes	Planned	Planned
AEM[4]	Manual?	Yes	Yes	(6)	(6)	?	No	?

Table 1. Summary of Refinement Scheme Capabilities at the Time of Press

"Planned" - discussions with developers indicate progress is underway on these items.
"?" – Not explicitly documented or demonstrated.

1. Within child grid that differs from parent grid.
2. Across parent-child interface.
3. Not in the public domain.
4. Not evaluated here.
5. Feasibility and scoping level discussions have been completed.
6. Supported in AEM codes but not to the authors' knowledge demonstrated in a parent-child type problem.

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