DT# 46977 QA:NA 2/15/06

New Ghost-Node Method for Linking Different Models with Varied Grid Refinement

Scott C. James¹, Jesse E. Dickinson², Steffen W. Mehl³, Mary C. Hill³, Stanley A. Leake²,
George A. Zyvoloski⁴, and Al-Aziz Eddebbbarh⁴

¹Sandia National Laboratories, PO Box 5800, Albuquerque, New Mexico, 87185-0735, USA:
scjames@sandia.gov

²U.S. Geological Survey, 520 N Park Suite 221 Tucson, Arizona, USA: jdickins@usgs.gov.

³U.S. Geological Survey, 3215 Marine St., Suite E-127, Boulder, Colorado, 80303, USA.

⁴Los Alamos National Laboratory, Group EES-6, MS T003, Los Alamos, New Mexico, 87545, USA.

Abstract

A flexible, robust method for linking grids of locally refined models constructed with different numerical methods is needed to address a variety of hydrologic problems. This work outlines and tests a new ghost-node model-linking method for a refined "child" model that is contained within a larger and coarser "parent" model that is based on the iterative method of Mehl and Hill (2002, 2004). The method is applicable to steady-state solutions for ground-water flow. Tests are presented for a homogeneous two-dimensional system that has either matching grids (parent cells border an integer number of child cells; Figure 2a) or non-matching grids (parent cells border a non-integer number of child cells; Figure 2b). The coupled grids are simulated using the finite-difference and finite-element models MODFLOW and FEHM, respectively. The simulations require no alteration of the MODFLOW or FEHM models and are executed using a batch file on Windows operating systems. Results indicate that when the grids are matched spatially so that nodes and child cell boundaries are aligned, the new coupling technique has error nearly equal to that when coupling two MODFLOW models (Mehl and Hill, 2002). When the grids are non-matching, model accuracy is slightly increased over matching-grid cases.

Overall, results indicate that the ghost-node technique is a viable means to accurately couple distinct models because the overall error is less than if only the regional model was used to simulate flow in the child model's domain.

Introduction

For many sites where flow of contaminated groundwater is a concern, local grid refinement is commonly used to achieve both improved boundary conditions and adequate resolution for areas of interest (Mehl and Hill, 2002; 2004). The ability to use different model codes to simulate different grid resolutions allows the modeling effort to take advantage of: 1) existing models that were constructed using different codes, 2) features of different codes important for the different resolutions and simulated processes, and (or) 3) the expertise of diverse groups of modelers. This work presents a method for local grid refinement of ground-water flow models using different codes

(numerical techniques). Accurate methods of local grid refinement have been developed that demonstrate the advantages of having regional (parent) and local (child) models communicate so that the solution depends upon both domains (e.g., Mehl and Hill, 2002; 2004; Schaars, 2003). In addition to linking distinct models, remaining issues that are of concern here are: 1) the importance of designing locally refined grids that match with the adjoining coarser grid, and 2) the method used to define hydraulic conductivity between parent and child grids.

Mehl and Hill (2002; 2004) showed that rigorous linking of embedded models is important because the common less-rigorous methods, such as one-way coupled telescopic mesh refinement, are prone to considerable error

and, of further concern, that errors are generally not detectable or quantifiable. In addition, errors between coupled models using the technique of Mehl and Hill (2002; 2004) are expected to increase when model nodes are not horizontally aligned (non-matching case of Figure 2b).

Previous work has examined up to two-dimensional systems with hydraulic conductivity fields that are either homogeneous or smoothly varying (e.g., von Rosenberg, 1982; Quandalle and Besset, 1983; 1985; Forsyth and Sammon, 1985; Edwards, 1996; and Peszyński et al., 1999) or two-dimensional systems with typical levels of heterogeneity (Mehl and Hill, 2002). One of the more promising methods is the shared-node iterative method outlined by Mehl and Hill (2002; 2004), which is an extension of the work of Székely (1999). The primary advantages of this method are its accuracy and flexibility. Accuracy has been demonstrated through extensive testing and flexibility was achieved because any part of an existing model can be refined with minimal alteration to the rest of the model. Mehl and Hill (2002; 2004) use the shared-node method to link parent and child models, both of which are constructed with MODFLOW. Here, we extend the basic ideas of the shared-node method to create a new ghost-node method to link parent and child models constructed using different codes. Specifically, we use the new ghost-node method to link a parent model constructed with MODFLOW to a child model constructed with FEHM.

The shared-node approach to local grid refinement requires nodes to overlap (Mehl and Hill, 2002; 2004). This restriction is troublesome when models have non-matching nodes. It is important to determine whether the error introduced by maintaining non-matching nodes is large enough that one or both grids should be redesigned to produce overlapping nodes at the interface between the parent and child grids. As an alternative, we propose a new ghost-node method that is related to the work of Leake and Claar (1999) that accommodates non-matching nodes. Simulations with matching and non-matching nodes are compared for a simple homogeneous system.

The work presented here is unique in that: 1) the numerical methods may be distinct (here, finite-difference and finite-volume numerical

techniques), and 2) model grids with non-matching nodes and cell boundaries are considered. This paper addresses both issues using a test case equivalent to that of Mehl and Hill (2002).

Methods

In this work, the parent model is constructed using the finite-difference code MODFLOW-2000 (Harbaugh et al., 1990), and the child model is constructed using the finite-volume code FEHM (Zyvoloski et al., 1997). Both MODFLOW and FEHM have a specified hydraulic conductivity (or permeability) for a cell, or control volume, that surrounds nodes where hydraulic heads are calculated.

The flow chart for model coupling shown in Figure 1 is based on the procedure developed by Mehl and Hill (2002; 2004) and has ten steps: 1) simulate the parent model for the entire domain; 2) interpolate parent heads onto ghost nodes; 3) relax the heads if not on the first iteration; 4) calculate the conductance between a ghost node and its corresponding child node (these conductances need only be calculated once and stored in a file); 5) simulate the child model subject to the relaxed heads from the parent model; 6) distribute child boundary fluxes across parent cell faces; 7) relax the fluxes if not on the first iteration; 8) check head and flux changes for convergence – convergence is achieved when the change of heads and fluxes between successive iterations is within specified tolerances; 9) if not converged, apply the relaxed fluxes from Step 7 to the parent model at locations corresponding to the boundaries of the child model – parent cells within the domain of the child model are inactive; and, 10) go to Step 2 until convergence is achieved.

The accuracy of the grid-coupling method for matching and non-matching grids was tested using a two-dimensional idealized test case. Head errors are presented as the L_1 norm of head error, which is the average of the absolute values of differences between simulated values and “true” values calculated with an analytic solution. Total parent error includes differences for all cells outside of the child area, whereas the total child error included values from all cells in the child model except for the cell containing the well at the center of the model.

Figure 1: Process to iteratively couple parent and child models.

Ghost-Node Method of Linking Models

The links between the parent and child models—specified-head boundary conditions to solve the child model and specified-flow boundary conditions for the parent model—are achieved by using intermediary head and flow values at ghost nodes.

Heads

External head-dependent boundary conditions for the child model are assigned at the ghost nodes. The ghost nodes, illustrated with open blue circles in Figure 2, are located within the parent model along a line that passes through cell centers of parent cells that lie along the model interfaces. The interface between models is typically not equidistant from the ghost and child nodes. Geometrically based interpolations are often used (Quandalle and Besset, 1985), although Mehl and Hill (2002) demonstrate a modest increase in accuracy when using Darcy-weighted interpolation. Because Darcy-weighted interpolation does not readily extend to three-dimensional problems, only linear interpolation is used in this work. Thus, heads at the ghost nodes are calculated by linear

interpolation of heads from adjacent parent cell centers along the interface.

Fluxes

In two dimensions, flows between child and ghost nodes are conceptualized as occurring through a flow area, which is an area coplanar with the interface between parent cells and child control volumes. For the matching case (Figure 2a), flow passes first through the child control volume with hydraulic conductivity, K_C , then into the parent cell with hydraulic conductivity, K_P , in series. Thus, the effective hydraulic conductivity of an area is:

$$K_{eff} = \frac{K_C K_P d}{K_P d_C + K_C d_P}, \quad (1)$$

where d_C and d_P are lengths within the child and parent portions of the sub-area, respectively, $d_C + d_P = d$. Flow through the area of a child cell is a function of conductance (per unit thickness), which is defined as

$$c = \frac{K_{eff} l}{d}, \quad (2)$$

where l is the perpendicular length of the area with hydraulic conductivity K_{eff} , and d is the distance between the child and ghost nodes. Flow (per unit thickness) to a ghost node is simply the head difference multiplied by the conductance

$$Q_{GN} = (h_{GN} - h_C) c, \quad (3)$$

where h_{GN} is the ghost-node (parent-interpolated) head and h_C is the head of the adjoining child node from the solution of the child model. For the matching case, flow to a parent cell is simply the sum of flows to ghost nodes within that parent cell.

For the non-matching case (Figure 2b), flows from a single child cell to multiple parent cells are managed by dividing the flow surface into sub-areas (differently shaded areas in Figure 2b) to distinguish portions of the surface that connect to different overlapped parent cells. When a child control volume borders multiple parent cells, then the flow distribution into each parent cell must be weighted based on an effective hydraulic conductivity of the materials in the child and parent models, and the overlap area of the of the parent cell face with the child control-volume face. Note that flow to a ghost

Figure 2: (a) matching and (b) non-matching alignment between red parent cells and blue child control volumes. Parent cell centers are solid red circles and child nodes are solid blue circles. Ghost nodes (open blue circles) are on a dashed green lines passing through centers of parent cells bordering model interfaces and are also directly across from child nodes.

node can be assigned to a parent cell that does not encompass the ghost node. In addition, flow from a child cell to a ghost node need not be assigned to the parent cell with the nearest cell

center. Finally, child nodes at model corners may be associated with two ghost nodes.

To accumulate flow to the parent cells in the non-matching case, all contributing flows to a parent cell are partitioned by the weight of the conductance of the sub-areas associated with each parent cell. For example, the green shaded area has flow from the child node to the parent cell

$$Q_P = (h_{GN} - h_C) \frac{c_1}{c_1 + c_2}, \quad (4)$$

where c_1 is the conductance calculated from l_1 , K_C , K_P , d_C , d_P , and d , and c_2 is the conductance calculated from l_2 , K_C , K_P , d_C , d_P , and d .

The sum from all contributing child cells yields the flow to each parent cell, which is based on hydraulic properties from both grids. This method of assigning flows conserves mass across the model interface on the basis of both grid geometry and hydraulic flow properties. Therefore, the ghost-node method exchanges head and flow boundary conditions that are spatially and hydraulically consistent with the grids of both models.

Implementation

A DOS batch file is used to iteratively couple the MODFLOW and FEHM models. The batch file: 1) runs executable files for the model software, 2) runs utilities that calculate boundary conditions, and 3) runs a utility to check for model convergence. After running the MODFLOW executable, a head utility code reads output from MODFLOW and generates an ASCII file with head boundary data in a format readable by FEHM. If not on the first iteration, the head utility under-relaxes the change in heads from the previous iteration by a user-specified value. An under-relaxation parameter of 0.5 was used in all simulations; however, no attempts were made to optimize this parameter. The batch file then runs the FEHM executable and FEHM uses the head ASCII file for the head-dependent boundary condition at ghost nodes. Next, the batch file enacts the flow utility code to read ASCII flow output from FEHM (comprising flow data to the ghost nodes), and distributes flows to MODFLOW cell centers. The flow utility code assembles an ASCII file that is an input file for the FHB1 package for MODFLOW (Leake and Lilly, 1997). If not on the first iteration, the flow utility code under-

relaxes the change in flows. Finally, the batch file calls a convergence utility code to calculate the maximum relative change in both heads and flows at all connections between the MODFLOW and FEHM models. If the maximum relative change is less than user-specified closure criteria, the model has converged and the batch file terminates. For this study, closure criterion for both heads and fluxes was 10^{-5} . If the closure criteria are not met, the batch file again executes MODFLOW and continues with model iterations.

Test Case Design

The two-dimensional flow domain shown in Figure 3 was simulated by using a steady-state, confined parent and child model and is similar to the model configuration used by Mehl and Hill (2002). Boundary conditions in the parent model were specified heads of 10 m along the left side, 1 m along the right side, and no-flow boundaries along the top and bottom. The parent model has a 15×15 grid and is 1,350 m on each side, which yield 90×90 m² cells. The hydraulic conductivity of both models is 0.25 m/s and is homogeneous and isotropic. The child model is contained entirely within the parent model at the center of the flow domain. In addition, the child model has a pumped well at the center ($x = 675$ m, $y = 675$ m) and withdrawal is 5.5 m³/s. The left and right child/parent interface boundaries are at $x = 450$ m and $x = 900$ m, respectively, and the top and bottom interface boundaries are at $y = 900$ m and $y = 450$ m, respectively. Different test cases have various child cell sizes that yield both matching and non-matching grids at the interface. The 18 child-model grid resolutions tested ranged from 13×13 to 47×47 , which produced parent:child refinement ratios that ranged from 2.6:1 to 9.4:1. Four of the resolutions result in matching grids: 3, 5, 7, and 9:1. Non-matching resolutions are 2.6:1, 3.4:1, 3.8:1, 4.2:1, 4.6:1, 5.4:1, 5.8:1, 6.2:1, 6.6:1, 7.4:1, 7.8:1, 8.2:1, 8.6:1, and 9.4:1. These simple test cases were used to evaluate simulation errors for model coupling with matching and non-matching grids.

Figure 3: Head contours and observation locations for the two-dimensional test case having 3:1 refinement. Constant-head boundaries are 10 m along the left side and 1 m along the right side. Withdrawal is 5.5 m³/s from a well at the center of the child model.

Results

The simulated flow system of the coupled two-dimensional test case may be compared to the analytic solution. Head contours are symmetrical about $y = 625$ m and decrease linearly from 10 m to 1 m from left to right, and include a cone of depression around the well at the center of the model. The solution has greater resolution near the pumped well due to the refinement of the child model, which results in smoother contours near the well than would be achieved with only the coarse parent model.

Figure 4 indicates that the L_1 norm error of both the parent and child models decreases for increasing grid refinements from about 3.65×10^{-3} m in the parent model for a 3:1 refinement ratio to about 3.30×10^{-3} m in the parent model for a 9.2:1 refinement ratio. The error in the child model decreases from 1.92×10^{-2} m for a 2.6:1 refinement ratio to about 1.25×10^{-2} m for a 9.2:1 refinement ratio. The L_1 norm errors for the child models are larger than the errors for the parent models because the head solution within the child domain is more complex due to the steep head gradients caused by pumping. Both the child and parent model errors decrease for increasing refinement ratios because the improved

accuracy of the child model benefits the solution of the parent model through application of more accurate boundary conditions. In addition, matching child models have increased L_1 norm errors compared to neighboring non-matching refinements. This is a result of non-matching grids having more child cells in connection with the parent cells, which results in boundary condition information being passed to the parent model from a greater spatial extent (e.g., what occurs for higher order interpolation). The L_1 norms of head errors for these test cases are nearly equal to the error reported by Mehl and Hill (2002) for linking two MODFLOW models.

Figure 4: Head errors of the parent and child models for two-dimensional test cases.

Conclusions

The iterative grid-coupling method requires that the parent and child model communicate boundary condition data to improve the other's solution. It is considered successful because the overall error is less than if only the regional model was used to simulate flow in the child model's domain. Thus, the method provides a valuable new tool for linking models of different grid refinement to estimate ground-water flow. Finally, this work demonstrates that accurate solutions can be obtained from both matching and non-matching grids when coupling finite-difference (MODFLOW) and finite-volume (FEHM) numerical methods.

Acknowledgments

This work was supported by the Yucca Mountain Site Characterization Office as part of the Civilian Radioactive Waste Management Program, which is managed by the U.S. Department of Energy, Yucca Mountain Site

Characterization Project. Sandia National Laboratories is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

References

- Edwards, M. G., 1996, Elimination of adaptive grid interface errors in the discrete cell centered pressure equation. *Journal of Computational Physics*, **126**, 356–372.
- Forsyth, P. A. and P. H. Sammon, 1985, Local mesh refinement and modelling of faults and pinchouts. Paper SPE 13524, presented at: *The 8th SPE Symposium on Reservoir Simulation*, Dallas, TX, 267–278.
- Harbaugh, A. W., E. R. Banta, M. C. Hill, and M. G. McDonald, 1990, MODFLOW-2000, The U.S. Geological modular ground-water model—User guide to modularization concepts and the ground-water flow process. *U.S. Geological Survey Open-File Report 90-392*.
- Leake, S. A. and D. V. Claar, 1999, Procedures and computer programs for telescopic mesh refinement using MODFLOW. *U.S. Geological Survey Open-File Report*, 99-238.
- Leake, S. A. and M. R. Lilly, 1997, Documentation of a computer program (FHB1) for assignment of transient specified-flow and specified-head boundaries in applications of the modular finite-difference ground-water flow model (MODFLOW). *U.S. Geological Survey Open-File Report*, 97-571.
- Mehl, S., and M. C. Hill, 2002, Development and evaluation of a local grid refinement method for block-centered finite-difference ground-water models using shared nodes. *Advances in Water Resources*, **25**, 497–511.
- Mehl, S. and M. C. Hill, 2004, Three-dimensional local grid refinement for block-centered finite-difference groundwater models using iteratively coupled shared nodes: a new method of interpolation and analysis of errors. *Advances in Water Resources*, **27**, 899–912.

Peszyńska, M., Q. Lu, and M. F. Wheeler, 1999, Coupling different numerical algorithms for two phase fluid flow. In: *MAFELAP Proceedings of Mathematics and Finite Elements Applications*, Uxbridge, UK, 205–214.

Quandalle, P. and P. Besset, 1983, The use of flexible gridding for improved reservoir modeling. Paper SPE 12239 presented at: *The 7th SPE Symposium on Reservoir Simulation*, San Francisco, CA, 51–60.

Quandalle, P. and P. Besset, 1985, Reduction of grid effects due to local subgridding in simulations using a composite grid. Paper SPE 13527 presented at: *The 8th SPE Symposium on Reservoir Simulation*, Dallas, TX, 295–305.

Schaars, F., P. Kamps, J. Hoogendoorn, K. Maas, 2003, MODGRID, Simultaneous solving of different groundwater flow models at various scales; An application to the groundwater model of the Amsterdam Dune Water Area. Proceedings of: *MODFLOW and More 2003: Understanding through Modeling*, Golden, CO.

Székely, F., 1999, Numerical modeling of drainage schemes in layered formations: A Kuwait City case study, *Ground Water*, 37(6), 879–883.

von Rosenberg, D. U., 1982, Local mesh refinement for finite difference methods. Paper SPE 10974 presented at: *The 57th Society of Petroleum Engineers Annual Fall Technical Conference*, New Orleans, LA.

Zyvoloski, G. A., B. A. Robinson, Z. V. Dash, and L. L. Trease, 1997, Summary of the models and methods for the FEHM application: A finite-element heat- and mass-transfer code. Los Alamos National Laboratory Report LA-13306-MS.