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MODFLOW-2005, The U.S. Geological Survey Modular Ground-Water Model—Documentation of the Multiple-Refined-Areas Capability of Local Grid Refinement (LGR) and the Boundary Flow and Head (BFH) Package

Chapter 21 of
Book 6, Modeling Techniques, Section A, Ground Water
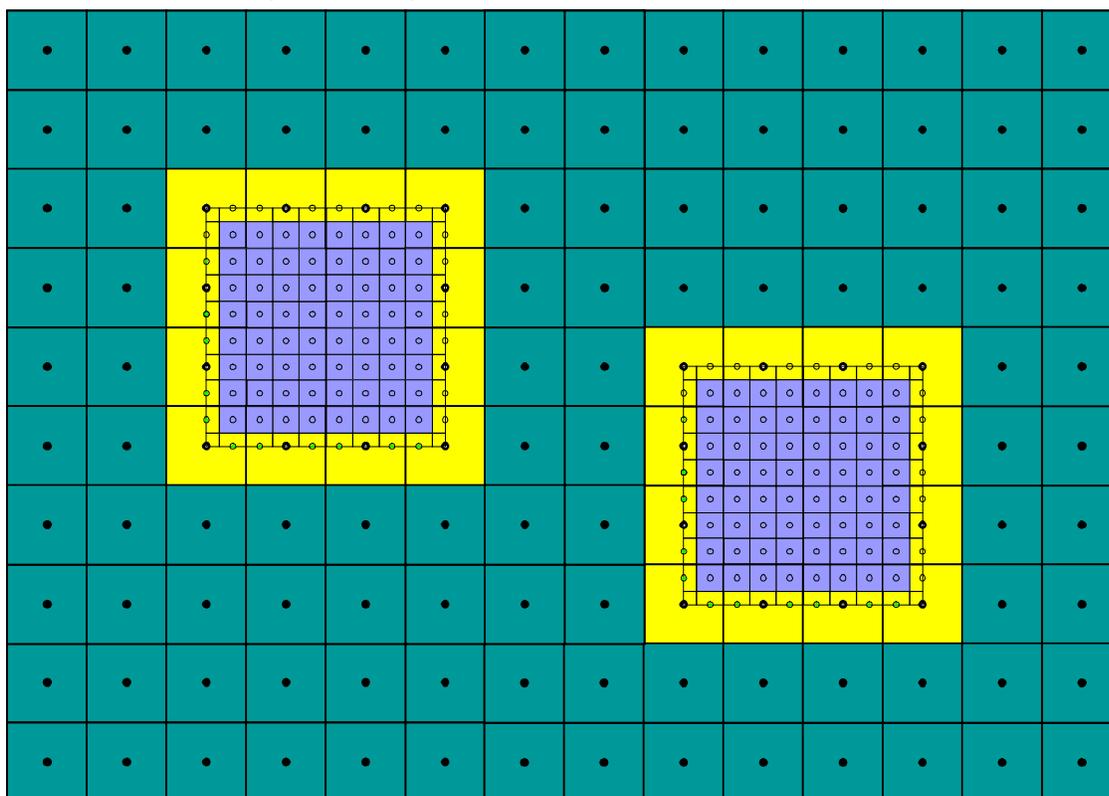
Techniques and Methods 6-A21

Cover: Schematic of two locally refined grids embedded within a coarse grid with detailed area showing the grid structure along the boundaries of the local grids.

MODFLOW-2005, The U.S. Geological Survey Modular Ground-Water Model—Documentation of the Multiple-Refined-Areas Capability of Local Grid Refinement (LGR) and the Boundary Flow and Head (BFH) Package

By Steffen W. Mehl and Mary C. Hill

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Suggested citation:
Mehl, S.W., and Hill, M.C., 2007, MODFLOW-2005, The U.S. Geological Survey modular ground-water model—Documentation of
the multiple-refined-areas capability of local grid refinement (LGR) and the boundary flow and head (BFH) package: U.S.
Geological Survey Techniques and Methods 6-A21, 13 p.

Preface

This report describes an addition to the shared node Local Grid Refinement (LGR) for MODFLOW-2005, the U.S. Geological Survey's three-dimensional finite-difference ground-water model. LGR is designed to allow users to create MODFLOW simulations by using a refined grid that is embedded within a coarser grid. This report extends that capability to allow multiple areas of refinement.

This report also describes the Boundary Flow and Head (BFH) Package for MODFLOW-2005, modified to accommodate the possibility of multiple areas of refinement. The BFH Package allows each refined grid to be run separately from the rest of the model, and the rest of the model to be run separately from the refined grids.

The performance of the programs has been tested in a variety of applications. Future applications, however, might reveal errors that were not detected in the test simulations. Users are requested to notify the U.S. Geological Survey of any errors found in this document or the computer program by using the e-mail address available at the Web address below. Updates might occasionally be made to both this document and to LGR and the BFH Package. Users can check for updates on the Internet at URL http://water.usgs.gov/software/ground_water.html/.

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Conversion Factors

Multiply	By	To obtain
meter (m)	3.281	foot
meter per second (m/s)	3.281	foot per second
square meter per second (m^2/s)	10.76	square foot per second
cubic meter per second (m^3/s)	35.31	cubic foot per second

Acronyms

LGR   Local Grid Refinement
BFH   Boundary Flow and Head

MODFLOW-2005, The U.S. Geological Survey Modular Ground-Water Model—Documentation of the Multiple-Refined-Areas Capability of Local Grid Refinement (LGR) and the Boundary Flow and Head (BFH) Package

By Steffen W. Mehl and Mary C. Hill

Abstract

This report documents the addition of the multiple-refined-areas capability to shared node Local Grid Refinement (LGR) and Boundary Flow and Head (BFH) Package of MODFLOW-2005, the U.S. Geological Survey modular, three-dimensional, finite-difference ground-water flow model. LGR now provides the capability to simulate ground-water flow by using one or more block-shaped, higher resolution local grids (child model) within a coarser grid (parent model). LGR accomplishes this by iteratively coupling separate MODFLOW-2005 models such that heads and fluxes are balanced across the shared interfacing boundaries. The ability to have multiple, nonoverlapping areas of refinement is important in situations where there is more than one area of concern within a regional model. In this circumstance, LGR can be used to simulate these distinct areas with higher resolution grids. LGR can be used in two-and three-dimensional, steady-state and transient simulations and for simulations of confined and unconfined ground-water systems. The BFH Package can be used to simulate these situations by using either the parent or child models independently.

Introduction

Simulations of ground-water flow and transport often need highly refined grids in local areas of interest to improve simulation accuracy. For example, refined grids may be needed:

(1) in regions where hydraulic gradients change substantially over short distances, as would be common near pumping or injecting wells, rivers, drains, and focused recharge; (2) in regions of site-scale contamination within a regional aquifer where simulations of plume movement are of interest; and (3) in regions requiring detailed representation of (hydro)geologic heterogeneity. Often, it is advantageous to refine more than one area of the model grid.

Refinement of the finite-difference grid used by MODFLOW-2005 (Harbaugh, 2005), the U.S. Geological Survey (USGS) modular three-dimensional, ground-water flow model, can be achieved by using globally refined grids, variably spaced grids, or locally refined grids, as discussed by Mehl and Hill (2005). The USGS Office of Ground Water and Ground-Water Resources Program, in cooperation with the Department of Energy, continued development of the shared-node local grid-refinement iterative method discussed by Mehl and Hill (2002, 2003, 2004) and Mehl and others (2006). One advantage of the shared-node local grid-refinement method is its ability to maintain continuity of flow and heads across the boundary between local (child) and regional (parent) grids without refining parts of the grid for which refinement is not desired. In

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addition, the parent and child models can be run either as a coupled system of models or separately, as independent models. The flexibility of being able to run the models separately can be very useful when, for example, solute transport within a refined grid is of interest.

Purpose and Scope

The purpose of this report is to document additions to MODFLOW-LGR and the Boundary Flow and Head (BFH) Package (Mehl and Hill, 2005). These additions allow users of MODFLOW-2005 (Harbaugh, 2005) to simulate multiple areas of grid refinement. This report first provides highlights of the new LGR (local grid refinement) capabilities. Next, the coupling strategy and opportunities for parallel execution are described and an example application is presented to demonstrate the performance of the program. Input instructions, example input and output, and important information to programmers are presented in the Appendix.

Acknowledgments

Highlights of New Capabilities

The updated version of LGR can simulate multiple areas of grid refinement, as shown in Figures 1 and 2. The following list of highlights is an addendum to those listed in the primary documentation of LGR (Mehl and Hill, 2005).

Coupling Strategy, Opportunities for Parallelization, and Execution Time

(1) In the iterative coupling strategy discussed in this report, all child grids are simulated before resimulating the parent grid with updated boundary conditions, as shown in Figure 1. That is, the effects of all child grids are accumulated and applied to the parent grid in a single parent simulation. In this approach, the ordering of the child-grid simulations does not affect the convergence or the results. An alternative coupling strategy would be to iterate between a parent-child pair before simulating the next parent-child pair. In this approach, the ordering of the parent-child simulations could affect model performance. It is conceivable that such a strategy might be advantageous in certain circumstances; however, such an iterative coupling strategy was not investigated and is not currently (2007) available.

(2) In the iterative coupling strategy used in this report, child model simulations can be executed independently of each other and, therefore, could be executed in parallel. However, parallelization of the child grid solutions is currently (2007) not implemented.

(3) LGR uses a solution method that iterates between the parent model and the child models. A single iteration requires one parent-model solution (execution time T_{parent}) and one child-model solution for each child model used (execution time $\bullet T_{child}$). The execution time per iteration is approximately the execution time of the parent grid, T_{parent}, plus the sum of the execution times for each child, $\bullet T_{child}$, which tends to cause a linear increase in execution time per iteration for each additional child model that is simulated. The number of LGR iterations required for convergence depends on the flow system being simulated. Experimentation so far has not indicated an increase in the number of LGR iterations when child grids are added.
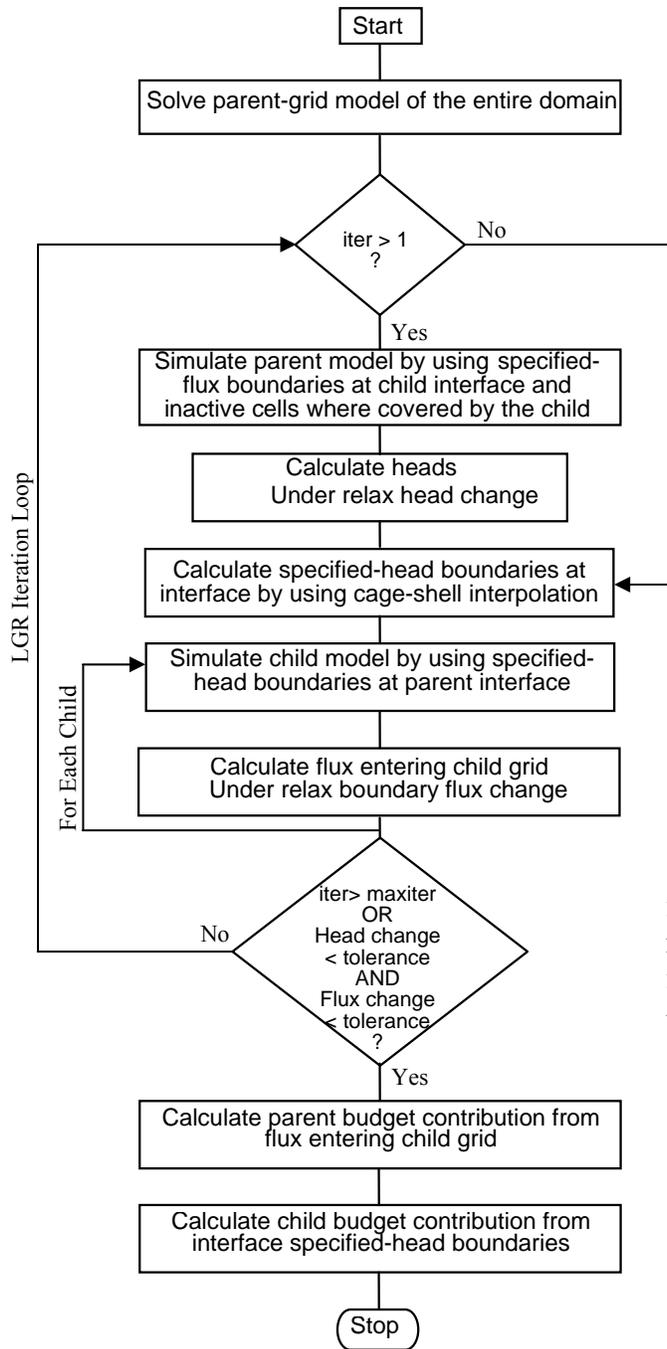
Figure 1. Flow chart for the iteratively coupled procedure with the modifications for multiple areas of local grid refinement labeled as "For Each Child."

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Model Grid Design

        The program documented in this report can simulate one or more block-shaped volumes of local-grid refinement. The refined areas cannot overlap, and at least one parent cell is needed between refined areas. Figure 2 shows an example with two parent-model grid cells between the two child model grids.
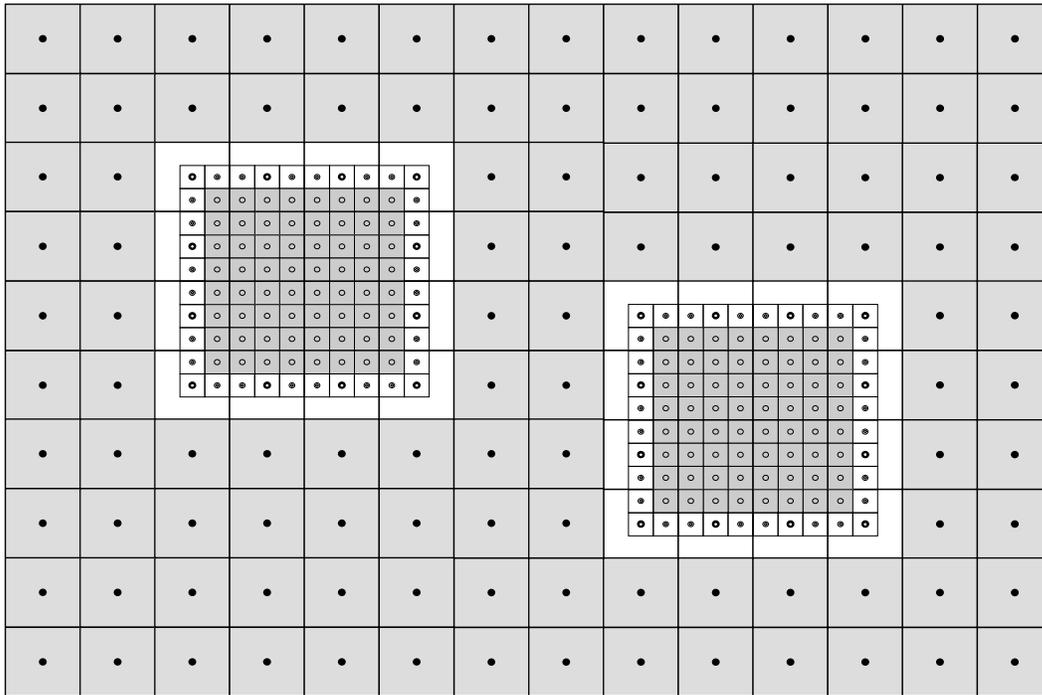
Figure 2. Schematic of a coarse grid with two areas of local grid refinement separated by two parent grid cells. At least one parent cell is required between child models.

        In three-dimensional models, different local grids can extend vertically to different levels of the parent grid. The vertical discretization needs to follow the same criteria described in Mehl and Hill (2006, p. 13).

Multiple Refined Areas Example

        A two-dimensional example is used to illustrate the multiple-refined-areas capability. Hydraulic head contours from this example are shown in Figure 3. This example is a modification of "example 1" described by Mehl and Hill (2005, p. 30). The parent model grid cells are 9.25 m by 9.0 m, which produces a grid that has 50 rows and 108 columns. The grid cells for both child models are 1.028 m by 1.0 m, representing a 9:1 refinement ratio. The modifications include the addition of a second pumping well of identical pumping rate (5.5×10^{-3} m^3/s), a homogeneous hydraulic conductivity field of 5.0×10^{-4} m/s, and constant-head boundaries of 10.0 m on the left and right sides. This test system was designed to have a symmetric flow field such that both child models have identical solutions while simulating different parts of the domain. This forms a test of the LGR program and, indeed, the solutions in the two grids were the same.
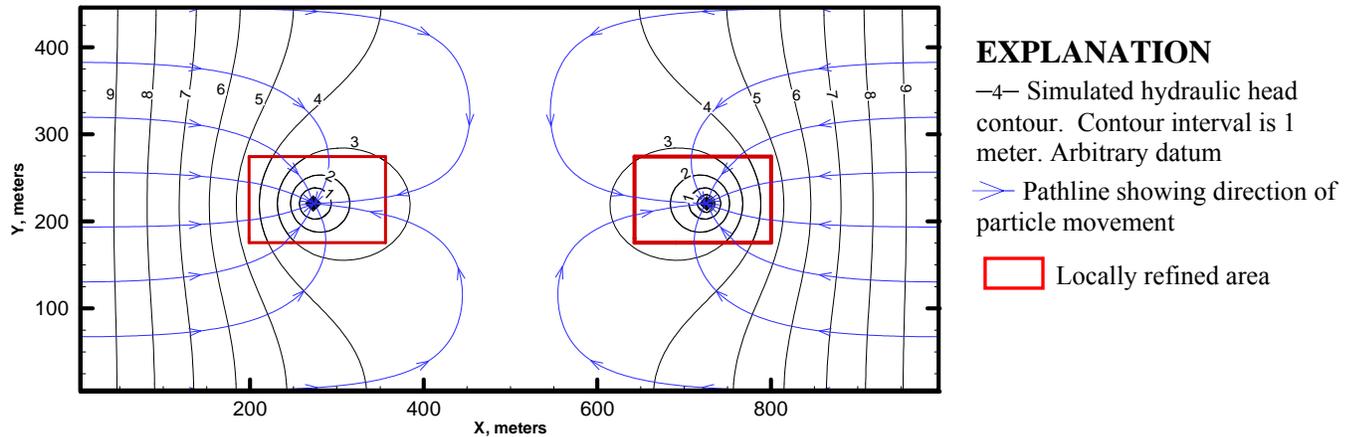
Figure 3. Example of grid refinement around two areas of pumping within a coarse-grid model. The system was designed to have a symmetric flow field.

Table 1 shows a comparison of the simulated hydraulic head at the wells and the computer processing times required for: (1) the coarse grid only, (2) the coarse grid coupled to the locally refined grids by using LGR, and (3) a globally refined grid. The globally refined grid uses the same grid spacing over the entire domain as the locally refined grids. The coarse grid coupled to the local grid by using LGR simulates a hydraulic head at the well that is in good agreement with the globally refined grid and requires somewhat less computer processing time. Approximately half the computer processing time (2.52 seconds) is required if only one area of refinement is simulated. This example demonstrates that the locally refined grids can improve the simulated drawdowns near the pumping wells (compared to the coarse grid), which is expected, and the approximately linear scaling of computer processing time when additional areas are simulated.

Though with the two local grids, the execution time is only reduced slightly in this problem; refining multiple areas in larger models is likely to be more computationally advantageous. Also, local refinement allows the rest of the model to remain unchanged. It also allows each of the models (here, the parent model or either of the child models) to be simulated independently, which can be advantageous when simulating computationally demanding transport processes.

Table 1. Comparison of simulated hydraulic head at the wells and computer processing time for several grids. Only one well is reported because the flow field is symmetric, as shown in Figure 3.

[Computation times using a Linux workstation, Pentium IV – 3.0 gigahertz]

Grid	Head at wells (meters)	Computer processing time (seconds)
Coarse	-3.11	0.055
Locally refined	-6.95	[1]4.82 (2.52)
Globally refined	-6.96	5.00

[1]With one area of refinement.

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References

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Mehl, S., and Hill, M.C., 2002, Development and evaluation of a local grid refinement method for block-centered finite-difference groundwater models using shared nodes: Advances in Water Resources, v. 25, no. 5, p. 497–511.

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Mehl, S.W., Hill, M.C., and Leake, S.A., 2006, Comparison of local grid refinement methods for MODFLOW: Ground Water, v. 44, no. 6, p. 792–796.

Appendix 1: LGR Input Instructions

When executed, MODFLOW-2005 prompts for the name of a file (the Name File; Harbaugh, 2005, p. 4-1 and 8-10). If a Name File is entered at the initial prompt, LGR is not used. To use LGR, enter the name of the LGR Control File at the initial prompt. The contents of this file are described here in full and are largely the same as the original input instructions described in Mehl and Hill (2005). Bold-face type is used to indicate relevant changes from the original input instructions.

The LGR Control File is distinguished from a Name File by the presence of a keyword "LGR" as the first non-commented input. LGR reads its input data from this file. Input for LGR is defined by using 15 items. Each item is read free format.

FOR EACH SIMULATION

0. [#Text]

Item 0 is optional – # must appear in column 1. Item 0 can be repeated multiple times.

1. LGR

2. NGRIDS

FOR THE PARENT GRID (the parent grid needs to be listed before the child grid)

3. NAME FILE

4. GRIDSTATUS

5. IUPBHSV   IUPBFSV

FOR **EACH** CHILD GRID [repeat items 6 through 15 for each grid with the exception of the parent grid. That is, repeat these items a total of (NGRIDS - 1) times]

6. NAME FILE

7. GRIDSTATUS

8. ISHFLG   IBFLG   IUCBHSV   IUCBFSV

9. MXLGRITER   IOUTLGR

10. RELAXH   RELAXF

11. HCLOSELGR   FCLOSELGR

12. NPLBEG   NPRBEG   NPCBEG

13. NPLEND   NPREND   NPCEND

14. NCPP

15. NCPPL [Repeat NCPPL a total of (NPLEND +1 – NPLBEG) times]

Explanation of Variables Read by LGR

LGR – the text "LGR" needs to be entered in the first item to indicate to MODFLOW-2005 that the LGR capability is used.

NGRIDS – is the total number of grids used in this simulation, including the parent grid and all of the child grids.

NAME FILE– is the name of the Name File for either the parent or child grid. The name can include the file path and is limited to 200 characters.

GRIDSTATUS – is a character variable and indicates whether the file listed in NAME FILE corresponds to a parent or child grid.

        If GRIDSTATUS = PARENTONLY, then it is a parent grid Name File.
        If GRIDSTATUS = CHILDONLY, then it is a child grid Name File.

IUPBHSV – A number greater than zero that corresponds to the unit number where the boundary heads are saved for later use by the BFH Package for independent simulations. A file with this unit number needs to be opened in the Name File of the parent model. A value of zero indicates that the file is not written. For the parent model, these are the complementary boundary conditions (see Appendix 2 of Mehl and Hill, 2005).

IUPBFSV – A number greater than zero that corresponds to the unit number where the boundary fluxes are saved for later use by the BFH Package for independent simulations. A file with this unit number needs to be opened in the Name File of the parent model. A value of zero indicates that the file is not written. For the parent model, these are the coupling boundary conditions (see Appendix 2 of Mehl and Hill, 2005).

ISHFLG – is a flag indicating whether heads from the parent grid simulation should be used as the starting head for the child grid simulation. These heads apply to the interior of the child, not the boundary.

        If ISHFLG = 1, then use results of the parent grid simulation as the starting head for the child grid. In the cells of the child grid that overlap the parent grid, the heads of the corresponding parent cell are used. No interpolation is applied. For steady-state simulations, this can provide a good initial guess which can reduce computational time. For transient simulations, this overwrites the initial condition of the child model defined in STRT of the Basic Package input file (Harbaugh, 2005) and, therefore, is not recommended.

        If ISHFLG = 0, then use the heads defined in STRT of the Basic Package for the child grid.

IBFLG – is a negative integer used to define the interface of the child grid with the parent. Use this value around the perimeter of the child model IBOUND array. Do not use IBFLG or -IBFLG anywhere else in the parent or child IBOUND arrays. **Use a unique value for each child grid.**

IUCBHSV – A number greater than zero that corresponds to the unit number where the boundary heads are saved for later use by the BFH Package for independent simulations. A file with this unit number needs to be opened in the Name File of the child model. A value of zero indicates that the file is not written. For the child model, these are the coupling boundary conditions (see Appendix 2 of Mehl and Hill, 2005).

IUCBFSV – A number greater than zero that corresponds to the unit number where the boundary fluxes are saved for later use by the BFH Package for independent simulations. A file with this unit number needs to be opened in the Name File of the child model. A value of zero indicates that the file is not written. For the child model, these are the complementary boundary conditions (see Appendix 2 of Mehl and Hill, 2005).

MXLGRITER – is the maximum number of LGR iterations; 20 iterations are sufficient for most problems. See Closure Criteria for LGR Iterations section of the report by Mehl and Hill (2005). Set MXLGRITER to 1 for a one-way coupling.

IOUTLGR – is a flag that controls printing from LGR iterations of the maximum head and flux change. For the maximum head change, the head value and corresponding layer, row, and column

of the child grid is listed. For the maximum flux change, the flux value and corresponding layer, row, and column of the parent grid is listed. If IOUTLGR < 0, output is written to the screen. If IOUTLGR > 0, output is written to the child listing file. If IOUTLGR = 0, no results are written.

RELAXH – is the relaxation factor for heads.

RELAXF – is the relaxation factor for fluxes.

Values of RELAXH and RELAXF less than 1 and greater than zero are needed for convergence of the LGR iterations. Typically, values around 0.5 produce convergent solutions. Values less than 0.5 may be needed when the LGR iterations have difficulty converging. In cases in which the LGR iterations exhibit no convergence difficulties, values greater than 0.5 may reduce the number of iterations needed for convergence. Convergence difficulties can be diagnosed by printing the maximum head and flux changes (IOUTLGR $\neq$ 0) to determine if the head and flux changes are decreasing (converging) or increasing (diverging) as the LGR iterations proceed.

HCLOSELGR – is the head closure criterion for the LGR iterations. The closure criterion is based on heads of the child-interface nodes. This closure criterion is satisfied when the maximum absolute head change between successive LGR iterations is less than HCLOSELGR (see equation 8b of the LGR documentation, Mehl and Hill, 2005).

FCLOSELGR – is the flux closure criterion for the LGR iterations. The closure criterion is based on fluxes into the parent-interface nodes. This closure criterion is satisfied when the maximum absolute relative flux change between successive LGR iterations is less than FCLOSELGR (see equation 8a of the LGR documentation, Mehl and Hill, 2005).

NPLBEG – is the number of the topmost layer of the parent grid where the child model begins. Currently (2007), refinement must begin at the top of the model so NPLBEG = 1.

NPRBEG – is the row number of the parent grid where the refinement begins (cannot equal 1).

NPCBEG – is the column number of the parent grid where the refinement begins (cannot equal 1).

NPLEND – is the number of the lowest layer of the parent grid where the refinement ends. NPLEND $\geq$ NPLBEG

NPREND – is the row number of the parent grid where the refinement ends. NPREND > NPRBEG and NPREND cannot equal the number of rows in the parent grid.

NPCEND – is the column number of the parent grid where the refinement ends. NPCEND > NPCBEG and NPCEND cannot equal the number of columns in the parent grid.

NCPP – The number of child cells that span the width of a single parent cell along rows and columns. This must be an odd integer number > 1 and is applied to rows and columns.

NCPPL – is the number of child cells that span the depth of a single parent layer. This must be an odd integer number $\geq$ 1. Read one value for each refined parent layer. The number of values needs to equals NPLEND +1 minus NPLBEG. Values can be 1, which results in no vertical refinement for the layer, only in layers above the bottom of the child grid, unless the refinement extends all the way to the bottom of the parent model (see The Top and Bottom of the Child Grid section of Mehl and Hill, 2005). For refinement that does not extend to the bottom of the parent model, the refinement terminates at the shared node; for example, in Figure 5b of LGR documentation (Mehl and Hill, 2005) the values 5 3 would be needed.

Appendix 2: LGR Input File for Multiple Refined Areas Example Shown in Figure 3

The sample data inputs listed below are for the two-dimensional example described in the Multiple Refined Areas Example section of this report, and shown in Figure 3. This example has two local areas of refinement, both with 9:1 refinement ratios. The first area of refinement begins in layer 1, row 20, column 22 and ends in layer 1, row 31, column 39 of the parent grid. The second area of refinement begins layer 1, row 20, column 70 and ends in layer 1, row 31, column 87. The annotated LGR input file is:

```
LGR                     #LGR Keyword
3                       #NGRIDS
parent.nam    #NAME FILE
PARENTONLY    #GRIDSTATUS
70 71                   #Unit #'s for complementary and coupling B.C.
child1.nam    #NAME FILE for the first child grid
CHILDONLY               #GRIDSTATUS
1 -59 80 81             #ISHFLG, IBFLG, Unit #'s for complementary and coupling B.C.
15 0                    #MXLGRITER, IOUTLGR
0.50 0.50               #RELAXH, RELAXF
1.0E-5 1.0E-5           #HCLOSELGR, FCLOSELGR
1 20 22                 #Beginning layer, row, and column
1 31 39                 #Ending layer, row, and column
9                       #Horizontal refinement ratio
1                       #Vertical refinement ratio by Parent layer
child2.nam    #NAME FILE for the second child grid
CHILDONLY               #GRIDSTATUS
1 -39 90 91             #ISHFLG, IBFLG, Unit #'s for complementary and coupling B.C.
15 0                    #MXLGRITER, IOUTLGR
0.50 0.50               #RELAXH, RELAXF
1.0E-5 1.0E-5           #HCLOSELGR, FCLOSELGR
1 20 70                 #Beginning layer, row, and column
1 31 87                 #Ending layer, row, and column
9                       #Horizontal refinement ratio
1                       #Vertical refinement ratio by Parent layer
```

LGR Input File Showing Available Flexibility

The sample data inputs listed below are for a three-dimensional example with two areas of refinement. This example demonstrates the available flexibility in that refinement ratios and convergence criteria can be different for each child grid. The first area of refinement begins in layer 1, row 20, column 22 and ends in layer 2, row 31, column 39 of the parent grid and uses a 9:1 refinement ratio horizontally and a 5:1 ratio of refinement vertically. The second area of refinement begins layer 1, row 6, column 22 and ends in layer 2, row 17, column 39 and uses a 3:1 refinement ratio horizontally and a 5:1 and 3:1 ratio of refinement vertically for the first and second parent layers, respectively. The annotated LGR input file is:

```
LGR                      #LGR Keyword
3                        #NGRIDS
ex2_parent.nam           #NAME FILE
PARENTONLY       #GRIDSTATUS
70 71                    #Unit #'s for complementary and coupling B.C.
ex2_child1.nam           #NAME FILE for the first child grid
CHILDONLY                #GRIDSTATUS
1 -59 80 81              #ISHFLG, IBFLG, Unit #'s for complementary and coupling B.C.
25 -1                    #MXLGRITER, IOUTLGR
0.50 0.50                #RELAXH, RELAXF
1.0E-5 1.0E-5            #HCLOSELGR, FCLOSELGR
1 20 22                  #Beginning layer, row, and column
2 31 39                  #Ending layer, row, and column
9                        #Horizontal refinement ratio
5 5                      #Vertical refinement ratio by Parent layer
ex2_child2.nam           #NAME FILE for the second child grid
CHILDONLY                #GRIDSTATUS
1 -39 90 91              #ISHFLG, IBFLG, Unit #'s for complementary and coupling B.C.
15 0                     #MXLGRITER, IOUTLGR
0.40 0.30                #RELAXH, RELAXF
1.0E-4 1.0E-4            #HCLOSELGR, FCLOSELGR
1 6 22                   #Beginning layer, row, and column
2 17 39                  #Ending layer, row, and column
3                        #Horizontal refinement ratio
5 3                      #Vertical refinement ratio by Parent layer
```

LGR Output

The output for each grid is the same as that shown by Mehl and Hill (2005, p. 56-58) for the case of a single refined area.

Appendix 3: Variables added to LGR to Simulate Multiple Areas of Refinement

Additional Variables in Fortran Module LGRMODULE

There are three new variables in LGRMODULE. They are listed in Table 2.

Table 2. Additional variables in Fortran module LGRMODULE.

Variable Name	Size	Description
NPLAY	Scalar	Number of layers in the parent grid
IBSHRD	Number of child boundary nodes	Array of flags for the child interface cells that indicates if the cell is a shared node (IBSHRD = 1) or not (IBSHRD = 0). The index is defined by looping through the child interface cells in the order of columns, rows, and layers.
IBPFLG	Number of grids	A list of IBOUND flags (IBFLG) used within this grid.

Additional Variables in Fortran Module GWFBFHMODULE

There are three new variables in GWFBFHMODULE. They are listed in Table 3.

Table 3. Additional variables in Fortran module GWFBFHMODULE.

Variable Name	Size	Description
NGRIDS	Scalar	Number of grids simulated.
IBSHRD	Number of child boundary nodes	Array of flags for the child interface cells that indicates if the cell is a shared node (IBSHRD = 1) or not (IBSHRD = 0). The index is defined by looping through the child interface cells in the order of columns, rows, and layers.
IBPFLG	Number of grids -1	A list of IBOUND flags (IBFLG) used within this grid.