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Simulation of Groundwater Flow based on Adaptive Mesh Refinement

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Abstract: The simulation of groundwater flow based on numerical methods requires sufficient discretization in areas of the domain where large changes of the hydraulic head gradient are expected. Mesh generation is the first step of numerical modeling, whereby the domain is discretized into a mesh of elements. The density of the mesh is defined prior to the simulation based primarily on user experience. In addition, a priori mesh generation for non-linear unconfined flow problems becomes very inefficient as there is no information regarding the water table. To alleviate the subjective and experimental mesh generation procedure in non-linear problems we propose a coupled scheme which combines adaptive mesh generation with a non-linear solver. Starting with a very coarse initial mesh, the mesh nodes are modified after every iteration of the non-linear solver so that the top boundary is equal with the hydraulic head. In addition, a refinement/coarsening step is executed where certain cells with very large or very small errors are refined or coarsened, respectively. The method is applied to a two dimensional hypothetical aquifer using three different distributions of hydraulic conductivity. The results show that the method is capable of producing optimized meshes by adding necessary degrees of freedom. In addition the non-linear problem converges during the first iterations when the mesh is coarser thus a faster convergence is achieved.

Keywords: Groundwater flow; Adaptive mesh refinement; Posteriori error estimation; Non-linear simulations; Unconfined aquifers.

1. INTRODUCTION

In groundwater hydrology, numerical models are used to simulate the flow and analyze future behavior of aquifer systems in response to management changes or changes in aquifer stresses. Spatial and temporal discretization converts the partial differential equations into a system of linear equations. The two most commonly used discretization methods are finite difference and finite element methods. In finite difference methods the domain is spatially discretized to a grid of rectilinear cells; in finite element methods the domain can be discretized into elements of various types and sizes. In finite element methods, the element size may vary locally without affecting the overall mesh, unlike in a finite difference mesh. Thus, finite element methods are better suited for applications with abrupt local changes in the flow field and highly irregular domains.

The size of mesh elements depends on factors such as the geometry of the domain, but more importantly on the solution of the partial differential equation. Generally the mesh element size is tightly connected with the divergence of the solution. The greater the solution divergence (change in gradient) is, the smaller elements (or time-steps) are needed to accurately reproduce the true solution. In groundwater flow simulations the element size is typically smallest near flow sources and sinks, e.g. wells, rivers, and in areas with abrupt changes of hydraulic properties.

Modeling platforms generally provide options to create varying element size meshes. But users are required to choose appropriate settings before the simulation. For example, consider the simulation of flow around a pumping well. Hydraulic head gradients increase with proximity to the well. The user needs to decide the minimum element size around the well, the element size growth, i.e. how much the size of two adjacent elements can deviate and a maximum distance to which the element size growth rule applies. These parameters depend on factors such as pumping rate, hydraulic conductivity, and groundwater recharge and their estimation is a difficult task and subject to user experience. In addition when multiple wells are present, each well would require its own parameter set. Similar difficulties are true for all types of sources and sinks.

During mesh generation the users select the mesh parameters based on their experience. When the parameter set leads to very fine discretization, the simulation results are expected to accurately approximate the true solution, at the expense of increased computational burden. On the other hand if the mesh parameters lead to a relatively coarse discretization, the computational burden is small, however the simulation results may not be accurate.

To avoid a subjective choice of mesh generation, Adaptive Mesh Refinement (AMR) has been proposed. In AMR the simulation starts with an initial coarse mesh which is adaptively refined in areas where the hydraulic head gradient is expected to change rapidly. During AMR, the system is solved repeatedly starting with a very coarse mesh. Based on the solution of the previous mesh an error estimator is calculated for each cell. The cells with higher error are chosen for refinement, while it is possible that cells with small estimation error be chosen for coarsening.

In linear systems of equations such as confined groundwater flow, AMR seems to increase the computational burden because it involves a sequence of solutions. Nevertheless the first iterations are generally executed very fast because the initial mesh is coarse. Due to the lack of easy-to-use software that implement AMR, the applications of AMR in groundwater flow is quite limited (Cao and Kitanidis 1998; Cao and Kitanidis 1999; Dietrich et al., 2008). To the best of our knowledge there are not references where AMR is used for non-linear simulations of groundwater flow.

In this paper we use AMR for the simulation of unconfined flow which is a non-linear problem. Non-linear problems are solved iteratively until certain criteria are met. In this study, at each non-linear step, we perform two additional steps. The mesh is first modified so that the elevation of the top boundary nodes is equal to the hydraulic head and secondly refinement/coarsening step based on the solution of the previous iteration.

The following section describes the governing equations and how AMR is used for the simulation of non-linear unconfined problems. The third section illustrates an application of the proposed methodology and the last section summarizes the main findings of this study.

2. ADAPTIVE MESH REFINEMENT IN UNCONFINED AQUIFERS

The governing equation that describes the general groundwater flow is:

$$S_s \frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left(K_x \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial h}{\partial z}\right) + Q_s \qquad (1)$$

where h is the unknown hydraulic head, K_x, K_y, K_z are the components of hydraulic conductivity along the principal axis, Q_s represents the sources and sinks, S_s is specific storativity and t is time. In unconfined aquifers, under Dupuit-Forcheimer assumption (Bear 1979), the hydraulic conductivity is a function of the hydraulic head. Therefore after discretization, equation (1) is converted to a system of equations of the form $KH = F$, where the matrix K depends on the unknown hydraulic head H.To solve the non-linear problem we start with an initial guess for vector H, which is then used to compute an initial conductance matrix K. The system is solved and a new hydraulic head vector is computed, which is used to correct the matrix K. This process is repeated until the difference between two consecutive iterations is smaller than a threshold.

The first step in numerical simulations is the mesh generation. Mesh generation is a rather complex and subjective task because the mesh is constructed before the simulation. Hence the users choose mesh generation rules based on their experience so that the generated meshes follow the distribution of the solution function. Ideally, finer mesh should be generated where higher gradient is expected. In addition for non-linear problems the mesh may change after every iteration, which adds another degree of difficulty in setting rules for mesh generation before the simulation.

To alleviate the shortcomings of the a priori mesh generation methods we propose the use of adaptive mesh refinement. In AMR we start by generating a coarse mesh. In non-linear problems the initial distribution of unknown heads is estimated on the coarse mesh. The coarse problem is solved and based on the solution we compute an error estimation for each mesh element. The elements with large errors are split into smaller elements. It is also possible to join adjacent cells with very small error known as coarsening. In non-linear problems before refinement or coarsening, the mesh of the previous step is adapted based on the solution. In unconfined problems the elevation of top nodes which represent the water table should be equal to the hydraulic head. In this paper we modify the z-coordinates of the entire mesh according to the following formula:

$$Z^{new}(x,y) = (Z^{old}(x,y) - Z^{bot}(x,y))\frac{Z^{new}_{top}(x,y)-Z^{bot}(x,y)}{Z^{old}_{top}(x,y)-Z^{bot}(x,y)} + Z^{bot}(x,y) \qquad (2)$$

Where $Z^{new}(x,y)$ is the modified elevation, $Z^{old}(x,y)$ is the elevation of the node at the previous iteration, $Z^{new}_{top}(x,y)$ and $Z^{old}_{top}(x,y)$ are the elevations at the top boundary of the mesh at the coordinate (x,y), which are equal to hydraulic head, at the new and previous non-linear iteration. $Z^{bot}(x,y)$ is the elevation at the bottom boundary of the aquifer at the same location. It can be seen (Figure 1) that the elevations $Z^{new}_{top}(x,y)$, $Z^{old}_{top}(x,y)$ and $Z^{bot}(x,y)$ may not correspond to an actual mesh node. In that case the elevations are interpolated.

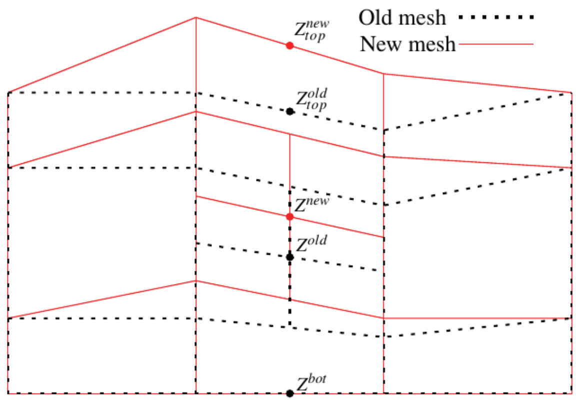

Figure 1 Explanation of symbols of mesh modification formula

A major issue in AMR methods is to estimate which cells should be refined or coarsen. To this end a number of criteria can be found in literature (Gratsch and Bathe 2005; Ainsworth and Oden 1997; Ainsworth et al., 2013). Here we employed a posteriori error estimator developed for the Laplace equation by Kelly et al., 1983 and it is given by:

$$\eta_K^2 = \frac{b}{24}\int_{\partial K}\left[\frac{\partial h_h}{\partial x} + \frac{\partial h_h}{\partial y} + \frac{\partial h_h}{\partial z}\right]^2 ds \qquad (3)$$

Where b is the element size, h_h is the discretized solution. After the computation of the error estimation for each cell we need to decide which cells should be refined/coarsen. To this end, the top T_f and bottom B_f fractions are defined, which determine how many cells will be marked for refinement or coarsening. Next the cell errors are sorted in decreasing order. Starting from the cells with higher errors we select a percentage of T_f cells with the largest errors for refinement and a percentage of B_f cells with the smallest errors for coarsening.

3. APPLICATIONS

The proposed coupled scheme of adaptive mesh refinement algorithm combined with a non-linear solver for the simulation of unconfined groundwater flow is applied to a two dimensional hypothetical flow problem. The implementation in three dimensions is straightforward because the model has been developed using the deal.ii (Bangerth et al., 2007) numerical library which adopts a dimension independent programming style.

The domain is rectangular with no flow boundaries on the right and bottom, constant head boundary on the left equal to 100 m, and constant flux boundary on the top equal with 0.5 m/day (Figure 2 left). The length of the aquifer is 1 km, therefore the total inflow from the top boundary is 500 m^3/day. In addition there is a well at x=500 m with screen length that extends vertically from the elevation of 30 m to 5 m with constant pumping rate at 500 m^3/day. The bottom of the aquifer is at -10 m and the initial water table is set equal to the elevation of 100m. Besides the sources and sinks the hydraulic properties of the porous medium can be very important factors in mesh generation. In this study we examine three different distributions of hydraulic conductivity.

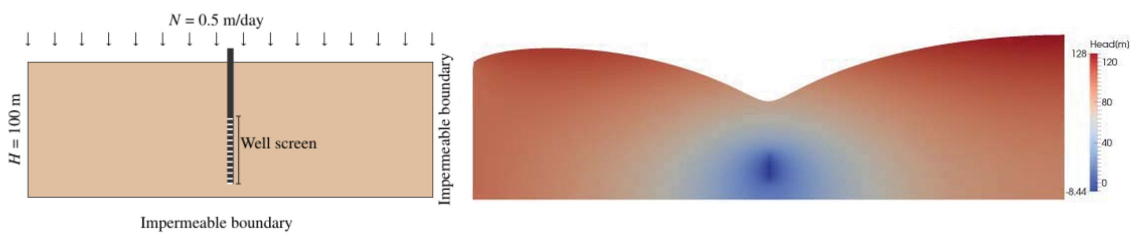

Figure 2. Left) Domain of the hypothetical example. Right) Homogeneous reference solution.

First we considered an homogenous aquifer with hydraulic conductivity along the x axis equal to K_{xx}=10 m/day, while the vertical component is equal to K_{zz}= 1 m/day. Initially the aquifer was discretized into a very fine mesh with element size equal to 1 m in x and z directions. However during the solution of the unconfined flow problem the element size along the z axis is expected to change. The distribution of hydraulic head is shown in Figure 2 (right). It can be seen that the water table has created a notable cone of depression above the screen length.

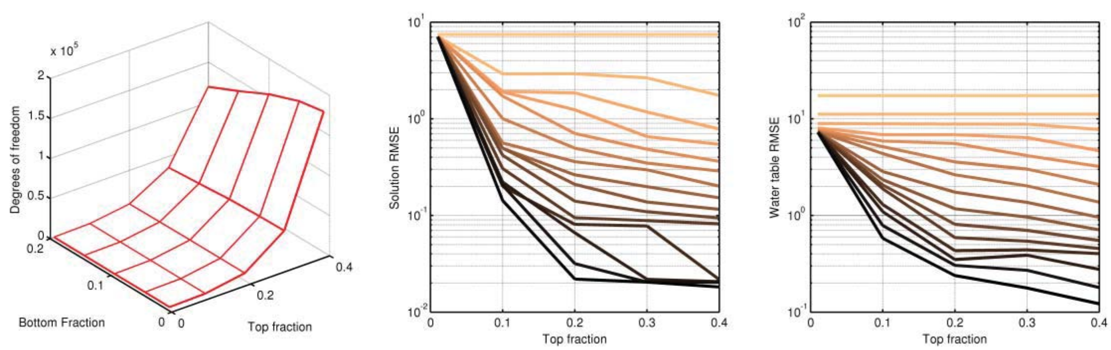

Figure 3. Sensitivity analysis of top and bottom fractions of adaptive mesh refinement. The left panel shows the degrees of freedom as function of top and bottom fractions. The middle and right panel shows the RMSE of solution and water table with respect to reference solution (Figure 2 left) as function of top fraction. Each color line corresponds to the RMSE at different steps. The lightest orange color line corresponds to initial step, while the black line corresponds to the final step of the non-linear solver

Next we simulated the hypothetical example using the AMR method starting from a very coarse mesh with 10 cells. The aquifer was simulated using all combinations of top T_f (1% 10% 20% 30% 40%) and bottom B_f (1% 5% 10% 15% 20%) fractions i.e. 25 simulations in total. The maximum number of iterations for the non-linear problem was set equal to 15. To compare the efficiency of each simulation we computed the root mean square error (RMSE) for a grid of points uniformly distributed in the aquifer domain between the solution at each non-linear iteration and the reference solution. In addition we computed the RMSE between the water table elevation every non-linear iteration and the reference water table.

In our example the top fraction T_f is more important factor for the accuracy of the solution compared to the bottom fraction B_f. As the top fraction increases more cells are refined each iteration, therefore the accuracy is expected to increase. On the other hand as the number of bottom fraction increases more cells will be chosen for coarsening. However the accuracy of those cells is already high therefore increasing or reducing the number of cells marked for coarsening has no significant loss of the accuracy but it has significant impact on the global number of degrees of freedom. It can be seen (Figure 3) that the degrees of freedom increases exponentially with the top fraction, while the degrees of freedom approximately decrease 32% when 20% of cells are selected for coarsening each iteration.

Figure 3 shows the comparisons between the simulation with AMR and the reference solution as function of the top fraction. Each different colour line corresponds to a different non-linear iteration. Initially the error is identical for all top fractions as it corresponds to the initial grid. For top fraction equal to 1% no cells are selected for refinement therefore there is no improvement of the accuracy. A limited improvement is achieved when 10% of the cells are used for refinement and the RMSE of the head distribution after 15 iterations is approximately 0.14 m, while the RMSE of the water table is 0.58 m. A significant improvement is achieved when 20% of the cells are selected for refinement each iteration. The error after 15 iterations is approximately 0.02 m and the RMSE of the water table is approximately 0.23 m. Finally further increase of top fraction does not result in significant reduction of the accuracy in this example.

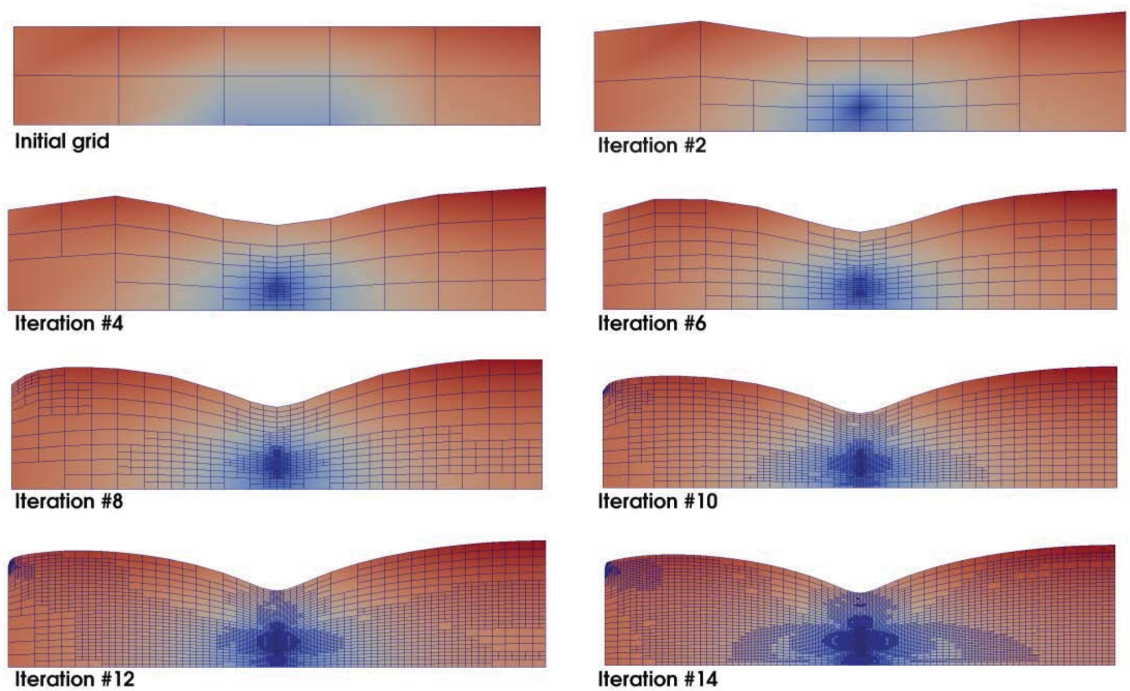

Figure 4. Mesh refinement with uniform hydraulic conductivity

Figure 4 shows the evolution of mesh refinement. During the first iterations the cells around the wells exhibit the greatest error based on the criterion (3). At the first iteration four cells were selected for refinement, the one that contains the well and the three neighbouring cells and each one is split into four child cells. In addition the nodes of the mesh are modified so that the top nodes represent the water table computed at the first iteration. At the second iteration another four cells, around the well, are selected for refinement. At the early iterations the mesh refinement focuses on the area around the well up to the 6-7 iteration, while the water table has been roughly approximated. After the 8^{th} iteration the criterion (3) identifies an area at the top left corner of the aquifer with error estimation comparable to the error around the well therefore during the subsequent iterations, cells of this area are also selected for refinement. We can also observe that after the 10th iteration the water table is very close to the reference water table.

In the next example we introduced an impermeable unit in the aquifer that extends along the x direction from 500 to 900 m and along z from 45 to 60 m. The sensitivity over the top and bottom fractions of AMR method is very similar to the uniform case. The RMSE of the solution after 15 iterations was 0.33 m and the water table approximation RMSE was approximately 0.65 and 0.35 for top fraction equal to 0.2 and 0.4 respectively.

Initially the cells with greater error estimation are those around the well. Nevertheless, as early as in the 3rd-4th iteration, the errors of the cells around the impermeable unit are comparable with the cell errors around the well. We can see that most of the cells along the impermeable unit have been refined at least once. After a small number of iterations (see Figure 5 iteration 8th) the impermeable unit has been clearly identified. Note that AMR method adds degrees of freedom only in areas where the head gradient exhibit large changes. We can see that the mesh is refined around the elevation 60 and 45 m while in between the mesh is coarser as there is no change in the head distribution within the impermeable unit. Similarly to the uniform case after the 8th iteration the AMR identifies cells with large errors near the top left boundary which refines during the subsequent iterations.

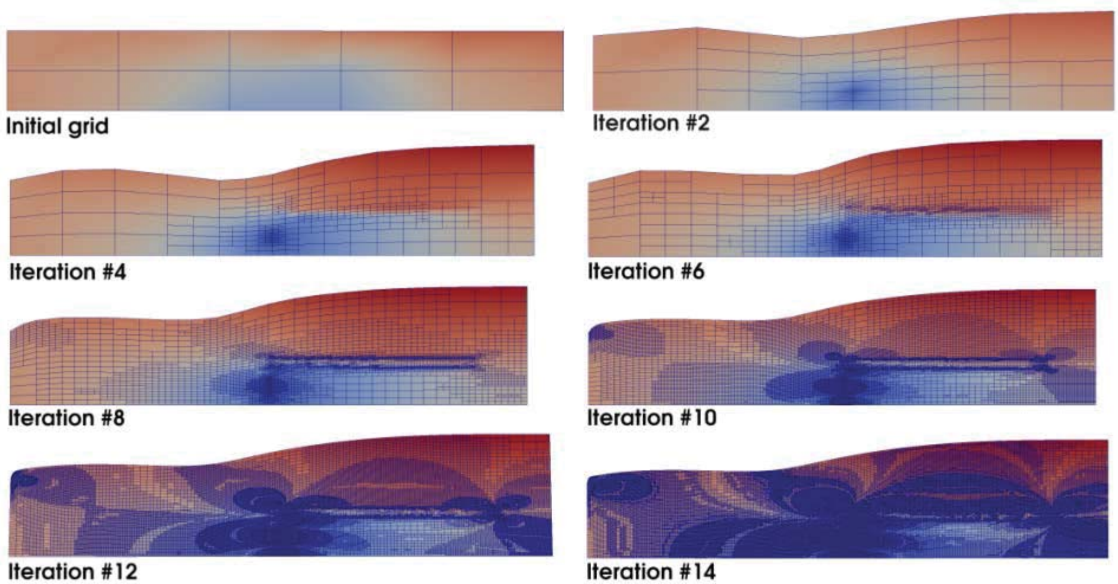

Figure 5. Mesh refinement with uniform hydraulic conductivity and an impermeable unit that extends along axis x: 500 -900 m and y:45-60 m.

Last we examine the effect of AMR method on a highly heterogeneous case where the logarithm of hydraulic conductivity distribution (Figure 6) is based on a Gaussian random field with mean $Log(K)$ =1.1 and standard deviation 0.2. This results in a lognormal distribution of hydraulic conductivity with values that span from 3 to 70 m/day with mean value 14 m/day.

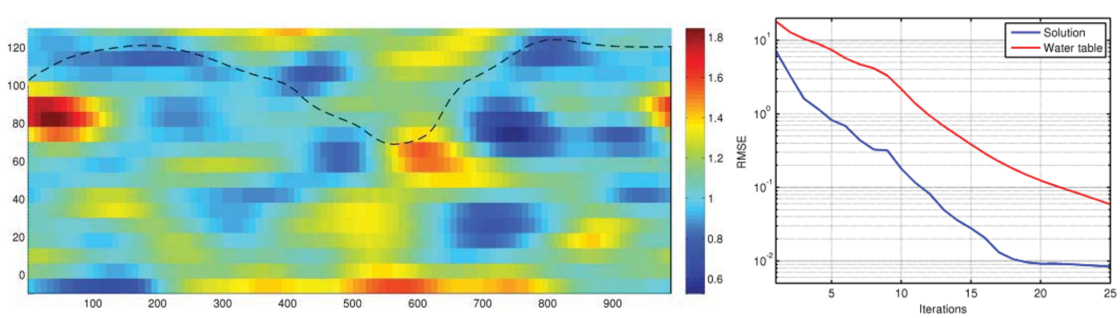

Figure 6 Left)Logarithm of hydraulic conductivity field based on Gaussian random field. The dashed line corresponds to the final position of the water table. Right) RMSE as function of iterations of non-linear solver.

The analysis over the values of the top and bottom fractions is similar to the other two cases. However in the heterogeneous case at least 18 iterations are needed for the solution to converge. The error was constantly reduced for 18 iterations while additional iterations did not result any further reduction of the RMSE. The RMSE appears to improve at every iteration for the water table Nevertheless the water table has been sufficiently approximated after 15th iteration (Figure 7). The gradient of the head distribution function even in the highly heterogeneous case is larger around the well. Therefore the cells around the well are marked for refinement during the first iterations. After the 6th iteration we observed that other areas of the aquifer start to be refined along with the area around the well. Due to the heterogeneity we observed that the cone of depression appears on the right of the well where the hydraulic conductivity has higher values (Figure 6 left). The shape of the water table has been clearly defined after 14 iterations, while most of the areas with significant gradient change have been refined after 18 iterations. The remaining iterations practically add unnecessary degrees of freedom.

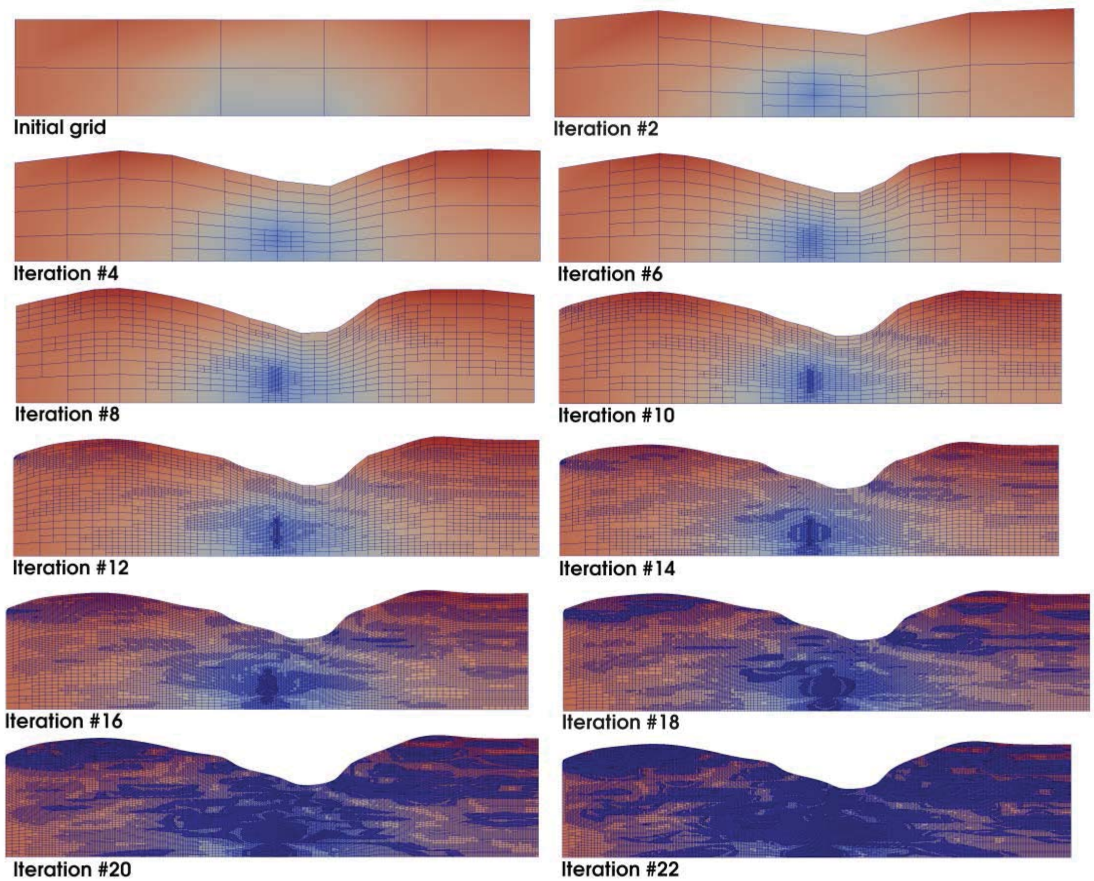

Figure 7 Mesh refinement based on the heterogeneous hydraulic conductivity distribution of Figure 6 left

4. CONCLUSIONS

In this paper we propose a coupled scheme for the simulation of unconfined aquifers. The method combines adaptive mesh refinement with a non-linear solver. Every iteration of the non-linear solver we perform a modification step and a refinement step. During modification, the mesh coordinates are adapted so that the nodes of the top layer coincide with the water table computed at the previous iterations. After the modification of the mesh the cells with greater errors are refined, while it is possible to coarsen cells with very small error. The approach has two distinct advantages:

(a) The first iterations where the main mesh modification occur are executed very fast because the mesh is quite coarse at the early iterations. Therefore the non-linear problem is solved first on relatively coarse mesh.
(b) We avoid subjective mesh generation rules, while the resulted mesh is optimized because the method introduces degrees of freedom where it is necessary.

The proposed method was applied to a two dimensional hypothetical flow problem under three different distributions of hydraulic conductivity. The results show that in homogenous or semi homogeneous cases fewer iterations are needed for the non-linear problem to converged compared to the highly heterogeneous case. The method was able to capture accurately the areas where higher changes of the gradient occurred.

Future research will focus on the development of appropriate stopping criteria as well as the extension of the method in transient state simulations where the mesh need to be adapted every time step

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