IMPROVED WELL MODELING TOOLS FOR UNSATURATED FLOW PUMP-AND-TREAT REMEDIATION STUDIES

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Abstract

Many Department of Defense military sites and Environmental Protection Agency superfund sites benefit from pump-and-treat systems for their remediation. One of the ways used to determine the effectiveness of a pump-and-treat system is by using a groundwater finite element method program to compute flow patterns from proposed well placement. As the governing Richards' equation for unsaturated flow is highly nonlinear, the finite element discretization often has trouble converging. This is especially true when (1) a significant part of the flow region has unsaturated flow, (2) the soils have relative hydraulic conductivities that go from almost vertical to almost horizontal, (3) water is being applied at the top of the flow region in very dry soil, and (4) wells become partially above the free surface when the pumping is turned on. This paper focuses on an improved well-modeling technique that allowed the finite element solution to go from nonconvergent to converging in 10 nonlinear iterations on the U.S. Army Engineer Research and Development Center (ERDC) Cray XT3 using 16 processor elements for the Higgins Farm Superfund site. The Higgins Farm Superfund site, which is approximately 75 acres in size and currently operated as a cattle farm, is located in a rural area along Route 518 in Franklin Township, Somerset County, New Jersey. The site is primarily pastureland where a drum burial dump was discovered. Extraction wells were placed around the perimeter with an onsite treatment plant. The finite element run not only did not converge but also the modeling of wells was initially very tedious. A given well has a specified flow, and the user would manually try to distribute this flow among the given set of nodes modeling the well. During the iteration toward nonlinear convergence, if a node of a well became above the free surface (pressure head less than zero), the code stopped. The user then manually redistributed the flow for that well and started the process again. However, combining all of the nodes for a well into one well supernode was determined to be the best solution. The nodes representing a partially penetrating well are combined into a single degree-of-freedom well supernode. Now, one total value of flow is used as input to the well supernode, and one single value of total head is computed as output. Both a reversible procedure and a nonreversible elimination of well nodes above the water table were implemented and studied. This paper will give the details of this computational experience using the high performance computers at the ERDC and discuss the general applicability of this approach to other studies.

1. Introduction

Many Department of Defense military sites and Environmental Protection Agency superfund sites benefit from pump-and-treat systems for their remediation. One of the ways used to determine the effectiveness of a pump-and-treat system is by using a groundwater finite element method program to compute flow patterns from proposed well placement. As the governing Richards' equation for unsaturated flow is highly nonlinear, the finite element discretization often has trouble converging. This is especially true when (1) a significant part of the flow region has unsaturated flow, (2) the soils have relative hydraulic conductivities that go from almost vertical to almost horizontal, (3) water is being applied at the top of the flow region in very dry soil, and (4) wells become partially above the free surface when the pumping is turned on. This paper focuses on an improved well-modeling technique that allowed the finite element solution to go from nonconvergent to converging in 10 nonlinear iterations on the U.S. Army Engineer Research and Development Center (ERDC) Cray XT3 using 16 processor elements (PEs) for the Higgins Farm Superfund site [*Environmental Protection Agency*, 1989].

2. Governing equations

Unsaturated flow in an isotropic soil is governed by

$$\nabla \cdot (k \nabla h) + \frac{\partial k}{\partial z} = \frac{\partial \theta}{\partial t} \tag{1}$$

where k is the hydraulic conductivity, h is the pressure head, z is the vertical coordinate, and θ is the moisture content. Since this particular study is a steady-state solution, the governing equation then becomes

$$\nabla \cdot (k \nabla h) + \frac{\partial k}{\partial z} = 0 \tag{2}$$

Hydraulic conductivity is modeled by

$$k = k_s k_r \tag{3}$$

where k_s is the saturated hydraulic conductivity, and k_r is the relative hydraulic conductivity. θ and k_r are both functions of h for unsaturated flow, thus creating a strong nonlinearity. For example, the relative hydraulic conductivity curves used in the Higgins Farm study for silty clay and fractured rock are given in Figure 1. The steep curves such as the one given in Figure 1 for silty clay are one of the main reasons why the numerical models have an extremely difficult time converging at times.

3. Higgins Farm

The Higgins Farm Superfund site, which is approximately 75 acres in size and currently operated as a cattle farm, is located in a rural area along Route 518 in Franklin Township, Somerset County, New Jersey. Figure 2 shows an April 1995 flyover with a red circle around the remediation site and the rock quarry shown in the lower left corner, and Figure 3 shows an aerial view of the remediation site and adjacent rock quarry. The

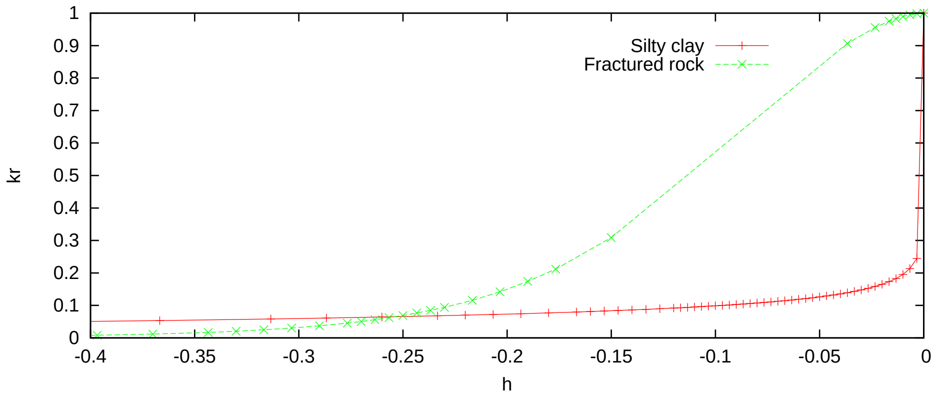

FIGURE 1. Relative hydraulic conductivity for silty clay and fractured rock

site is primarily pastureland. In 1985, the Franklin Township Health Department conducted sampling of a nearby residential well and found elevated levels of chlorobenzene. Subsequent investigations by the New Jersey Department of Environmental Protection (NJDEP) led to the discovery of a drum burial dump at the site approximately 40 yards from the contaminated well. In March 1987, NJDEP requested that the Environmental Protection Agency (EPA) assume the lead role for mitigating the site. In March 1989, the site was formally placed on the National Priorities List of EPA. The cleanup approach was addressed in two stages: (1) immediate action to provide affected residents with an alternate water supply and (2) a permanent long-term remedial action to address the groundwater contamination. Extraction wells were placed around the perimeter with an onsite treatment plant. One of the ways to help determine the effectiveness of this pump-and-treat system is to use a groundwater finite element method (FEM) program [*Donnell and Sanchez*, 2005].

4. Numerical model

The groundwater program FEMWATER [*Lin et al.*, 1997] was used in this study. It utilizes the standard Galerkin FEM with the capability to use three-dimensional (3-D) brick, prism, or tetrahedral elements. A Picard nonlinear solver and a conjugate gradient linear solver with a diagonal preconditioner were implemented to solve the nonlinear system of equations coming from the FEM discretization. A fully parallel version of FEMWATER [*Tracy*, 2000] using Message Passing Interface (MPI) for communication among PEs was created with METIS [*Karypis*, 2006] being used for partitioning the mesh. The Higgins Farm model in this study has 55,398 nodes and 101,764 3-D prism elements. Figure 4 shows a top view of the mesh. The initial computer run did not converge because of the severity of the slopes of the relative hydraulic conductivity curves as shown in Figure 1.

5. Well modeling

5.1. **Theoretical assumptions.** Classic modeling of a a well with a water table [*Cedergren*, 1968] is illustrated in Figure 5. The region where there is water in the well has a constant total head specified equal to the height of the water in the well. Between the

FIGURE 2. April 1995 flyover with a red circle around the remediation site and the rock quarry shown in the lower left corner

free surface and the the water height in the well is a surface of seepage that is neglected in this model. This area is very small in most regional groundwater simulations.

5.2. **Modflow.** Although new tools are in development, a well that extends into multiple layers is modeled in Modflow by having the user manually supply the well discharge for each layer. The recommendation that is made in the Modflow documentation [*McDonald and Harbaugh*, 1988, and *Harbaugh et al.*, 2000] for distributing the total well discharge among the layers is the result from assuming horizontal flow at the well as follows:

$$\frac{Q_i}{Q_w} = \frac{T_i}{T_w} \tag{4}$$

where Q_w is the total well discharge, Q_i is the well discharge for layer i, T_w is the total transmissibility of the well, and T_i is the transmissibility of layer i.

5.3. **FEMWATER.** Before the improvement, the modeling of wells in FEMWATER was very tedious. A given well has a specified flow, and the user would manually distribute this flow among the given set of nodes modeling the well (see Figure 6 where a well is modeled by the nodes given in Table 1 and are surrounded by a rectangular box in the

Figure 3. Aerial view of rock quarry and remediation site

figure and will be turned into a well supernode in the new scheme). During the nonlinear iteration process toward convergence, if a node of a well becomes above the free surface (pressure head less than zero), the code stopped. The user then manually redistributed the flow for that well among the remaining nodes below or on the free surface and started the computation again. Combining that tedium with the data set not converging clarified the need for an improvement.

5.4. **Well supernode.** Combining all of the nodes for a well into one well supernode was determined to be the best solution. The nodes representing a well are combined into a single degree-of-freedom well supernode. Now, one total value of flow is used as input to the well supernode, and one single value of total head is computed as output. Table 1 shows results for a given extraction well of the Higgins Farm computer run with the node numbers matching those in Figure 6. The input flows for each well of a well supernode are added in the program to determine the single input flow for that well supernode. There are two versions of the well supernode algorithm when some of the well nodes become above the free surface.

The first version converged in 10 nonlinear iterations on the ERDC Cray XT3 using 16 PEs. In this version, nodes that have negative pressure heads in a given well supernode (nodes 15790 and 19747 in Table 1) are left in the mesh. This creates nonrealistic flow values at these nodes (-0.54319 and -0.02753 instead of zero for each node) in that no flow is coming out at these nodes. However, this version is reversible in the nonlinear process.

A second version was created where the nodes with negative pressure head were removed from the well supernode and given a zero flow value. This version converged in 12 nonlinear iterations on the ERDC Cray XT3 using 16 PEs. It is important to note that the reason

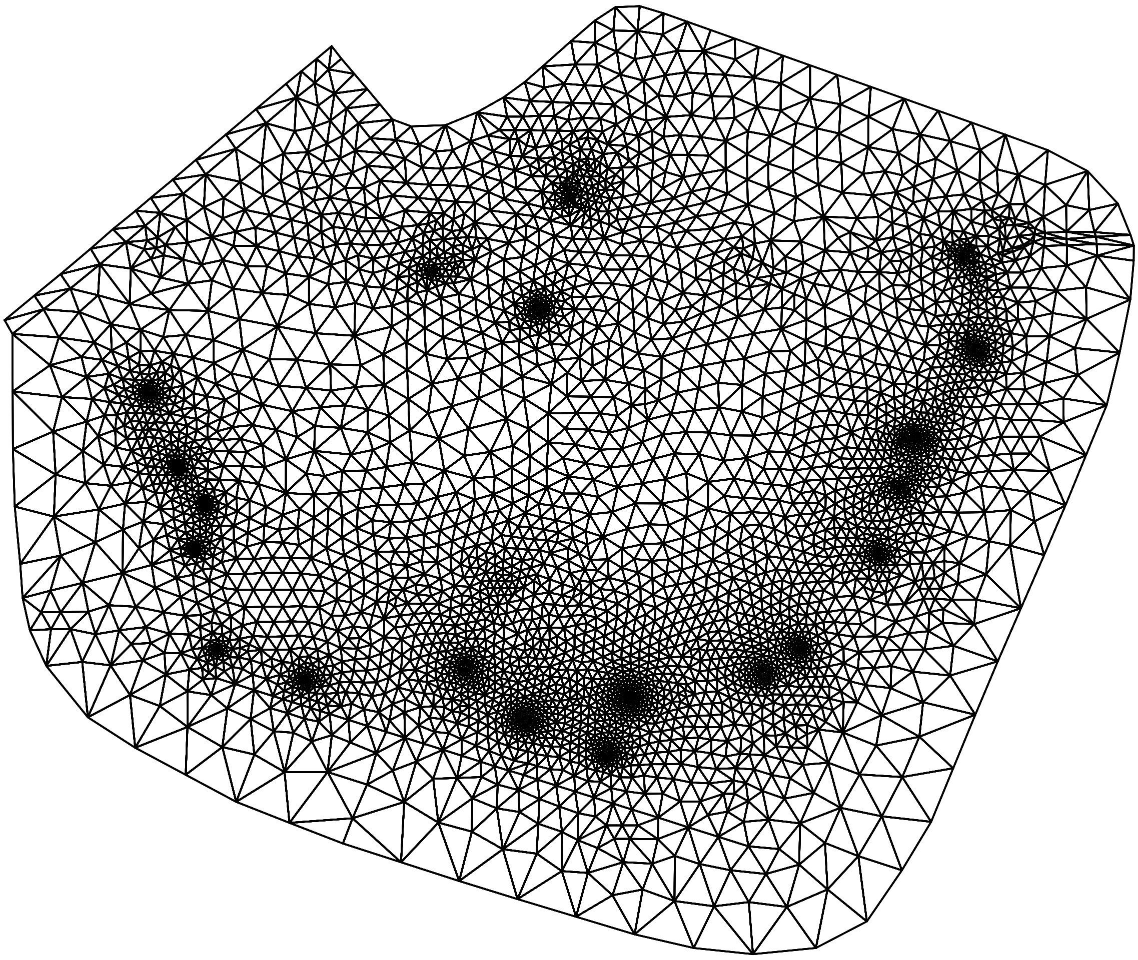

Figure 4. Top view of finite element mesh

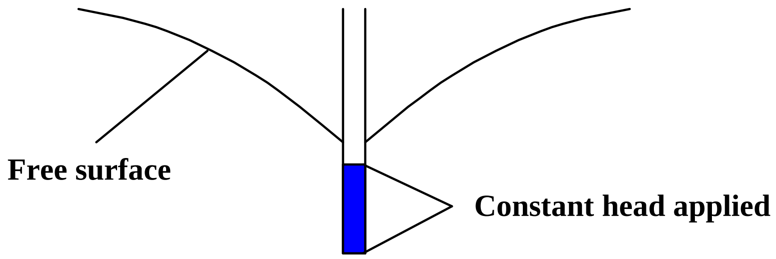

Figure 5. Partially penetrating well with free surface or water table

the flows for nodes 19747 and 15790 are not exactly zero is because the convergence criteria for the nonlinear process to stop is that the maximum change in pressure head be 0.001. So before Table 1 was computed, the material properties were updated one more time. Thus, the flows at the nodes above the water table will be slightly different from the original values (a measure of the quality of convergence). As seen at node 15790, once

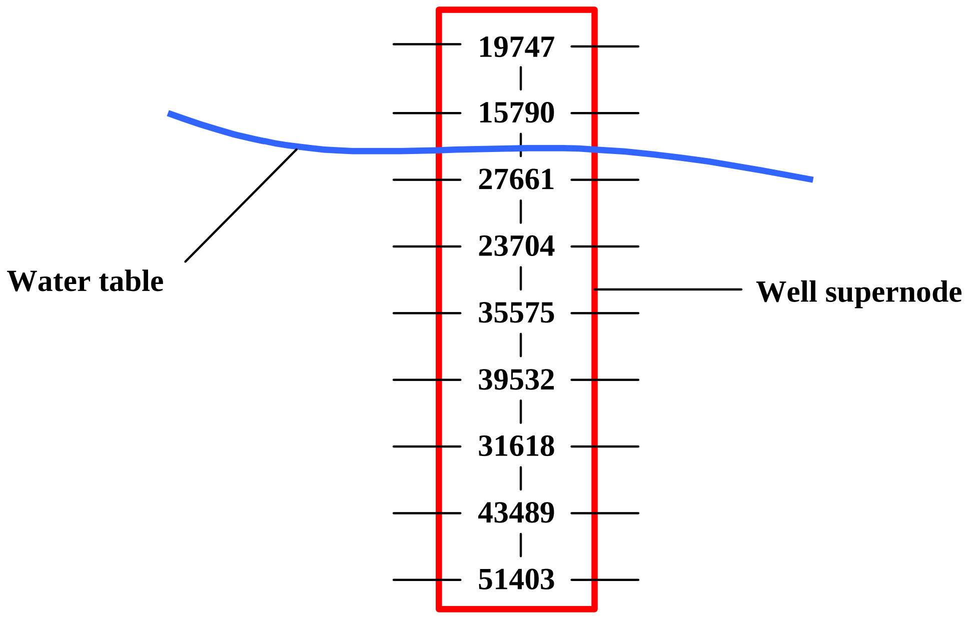

Figure 6. Modeling a well with a well supernode

Table 1. Results from a typical well supernode

Node	Input Q	Computed Q Version 1	Computed Q Version 2	z	h Version 1	h Version 2
19747	-0.25412	-0.02753	0.00024	253.792	-2.40948	-1.88970
15790	-0.71314	-0.54319	-0.00093	251.483	-0.10048	0.38933
27661	-0.99574	-0.97094	-1.20996	246.143	5.23952	5.22892
23704	-1.74109	-1.65519	-1.73843	240.804	10.57852	10.56793
35575	-2.48644	-2.33413	-2.38563	227.470	23.91252	23.90193
39532	-2.48644	-3.97871	-4.02473	214.137	37.24553	37.23493
31618	-3.10805	-4.54957	-4.59558	200.804	50.57852	50.56793
43489	-5.93027	-5.79844	-5.84815	180.804	70.57852	70.56792
51403	-9.32472	-7.18228	-7.23706	137.202	114.18053	114.16993
Total	-27.0400	-27.0400	-27.0402			

the flow is set to zero, the node can return to positive pressure head. If this node is then added back to the well supernode, it often will then compute a negative pressure head again. Thus, once a well supernode is removed, it must stay removed from the system to avoid this flip-flopping. Caution must be used in this option to make sure the nonlinear process has stabilized somewhat before starting the irreversible deleting of nodes.

6. Analysis and conclusion

When looking at the two sets of results, their differences are only very near the free surface, thus making them both a significant improvement over what was previously available. The pressure heads from the two versions at node 27661, for instance, which is just above the bottom two nodes, are 5.23952 and 5.22892, respectively, and are very close.

Furthermore, this technique is applicable to most other pump-and-treat simulations using the FEM whether the wells become in the unsaturated zone or not.

7. Acknowledgment

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