The Application of the Parallelized Groundwater Model FEMWATER to a Deep Mine Project and the Remediation of a Large Military Site

by

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Abstract

FEMWATER is a finite element method flow and transport groundwater model that has been parallelized under the Common High Performance Computing Software Support Initiative (CHSSI) project EQM-3 primarily in support of the cleanup of contaminated military sites. Last year at the HPC Users meeting the details of this effort were described. To show its high dual-use capabilities, parallel FEMWATER has been successfully applied to a deep mine project in support of Army civil works concerns this past year, as well as the traditional military application to help determine a successful remediation plan for a large military site. Results for the deep mine project and the large military site are given.

Unsaturated groundwater flow simulation is remarkably challenging because of the slowness of convergence of the resulting system of nonlinear equations. This paper first gives a brief description of the deep mine project and then concentrates on the further computational R&D needed to solve this real-world problem. On one of the DoD MSRC systems, 200 processing elements and approximately five hours of compute time were used to do thousands of time steps where one time step took four hours on a work station and three hours on a single node of one of the DoD MSRC systems. The large military site is then described and results for different solvers are given.

It is important to note that the Army civil works example chosen to highlight the capabilities of parallel FEMWATER is highly representative of the increased computing power that is now also available to military installations in support of site cleanup. Further, the paper will show that the calculations made to assess the effects of such subsurface problems would have been impossible to conduct at the resolution selected and level of sophistication of the science used in the absence of the DoD HPC resources.

Overview of Parallel (||) FEMWATER

FEMWATER (Lin, Richards, Talbot, Yeh, Cheng, Cheng, and Jones, 1997) is a 3-D finite element code to model saturated or unsaturated groundwater flow and contaminant transport. It can model a steady-state or transient analysis with either constant or variable density. Flow is done using the Galerkin method, and transport uses the Eulerian-Lagrangian method. || FEMWATER has five parts:

1. A C program to generate all needed include files and the QSUB file.

2. A C program to partition the grid using || METIS (Karypis, 1999).

3. A FORTRAN and C program to write files containing geometry, boundary conditions, and ghost data for each processing element (pe).

4. The || FEMWATER program written in FORTRAN.

5. The post-processor program written in FORTRAN to combine output files generated by each pe.

Note that the final results from || FEMWATER runs can be viewed and analyzed through the capabilities of the DoD Groundwater Modeling System (GMS) (Groundwater Modeling Team, 1999).

Deep Mine Project

Description of the problem

This deep mine project entails modeling the de-watering of a subsurface copper and zinc mineral deposits, and evaluating the impacts on wetlands and groundwater resources near the ore body location. The ore body is long and tubular with an approximate width of 100 feet north-south and a strike length of 4900 feet, east-west. The ore body begins at a depth of approximately 400 feet and extends to an approximate depth of 2200 feet beneath the surface. The purpose of the FEMWATER simulation of the proposed mining operation is to evaluate the results obtained from a more simplistic model developed by a differing group. Specifically, the model is to evaluate (1) the estimated rate of mine de-watering inflow; (2) the effects of the mine de-watering on regional groundwater flow; and (3) the effects of the mine de-watering on the streams, lakes, and wetlands water surfaces near the mine. Note that items 1-3 are indicative of the same information needed by decision makers in designing and operating a variety of remediation methods for military site cleanup. An aerial view of the project and mesh is given in Figure 1, and an isometric view of the 3-D mesh is given in Figure 2. Figure 3 shows drawdown, and Figure 4 shows total head continuous tone contours.

Computational constraints

The serial version of FEMWATER took approximately four hours on a large work station and three hours on a single node HPC system because of the highly nonlinear nature of the problem. However, 29 years of simulation were required, so thousands of time steps were required. Only the || version of FEMWATER could feasibly do this job. Given below are computational additions made to allow the successful completion of this phase of the study using 200 pe’s on the Cray T3E for approximately five hours.

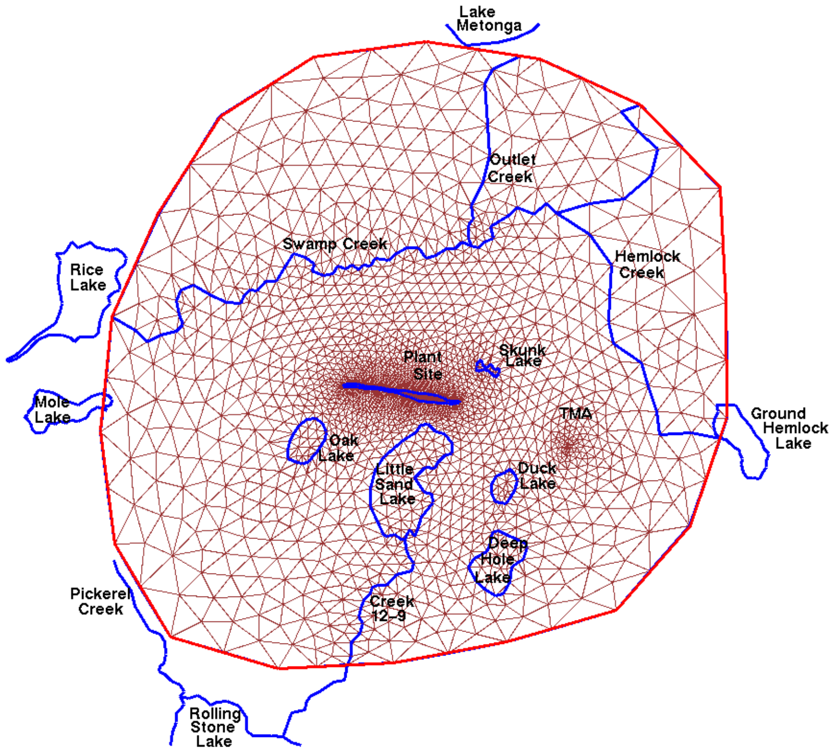

Figure 1. Aerial view of the deep mine project

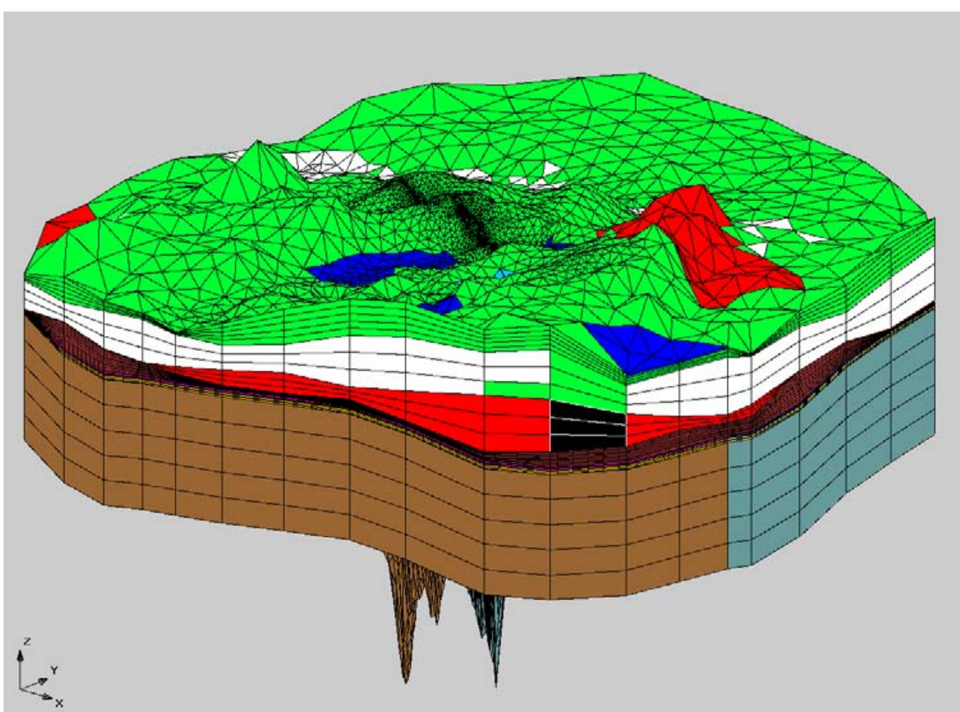

Figure 2. Isometric view of the deep mine project mesh

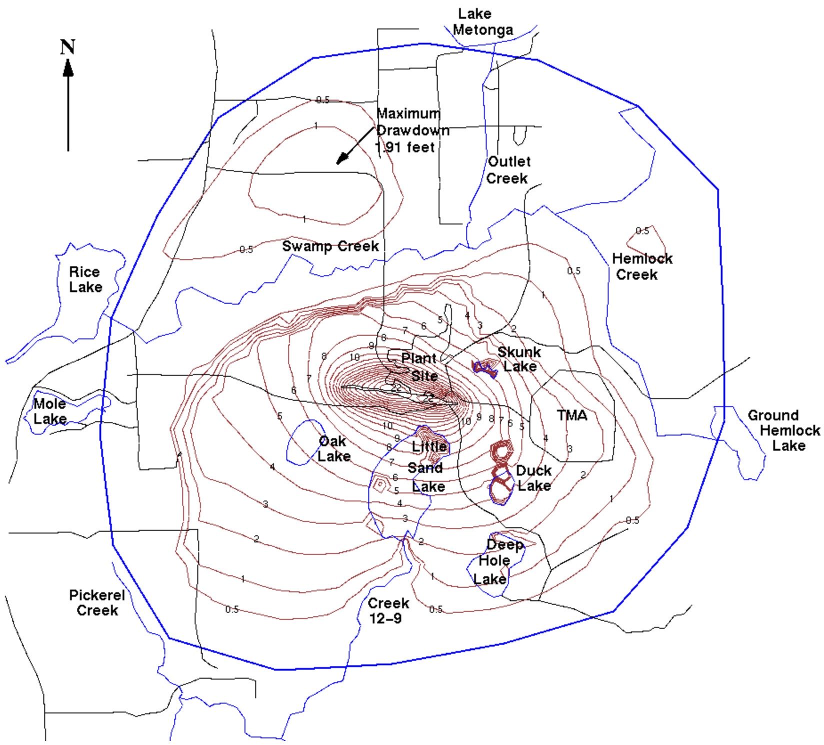

Figure 3. Drawdown

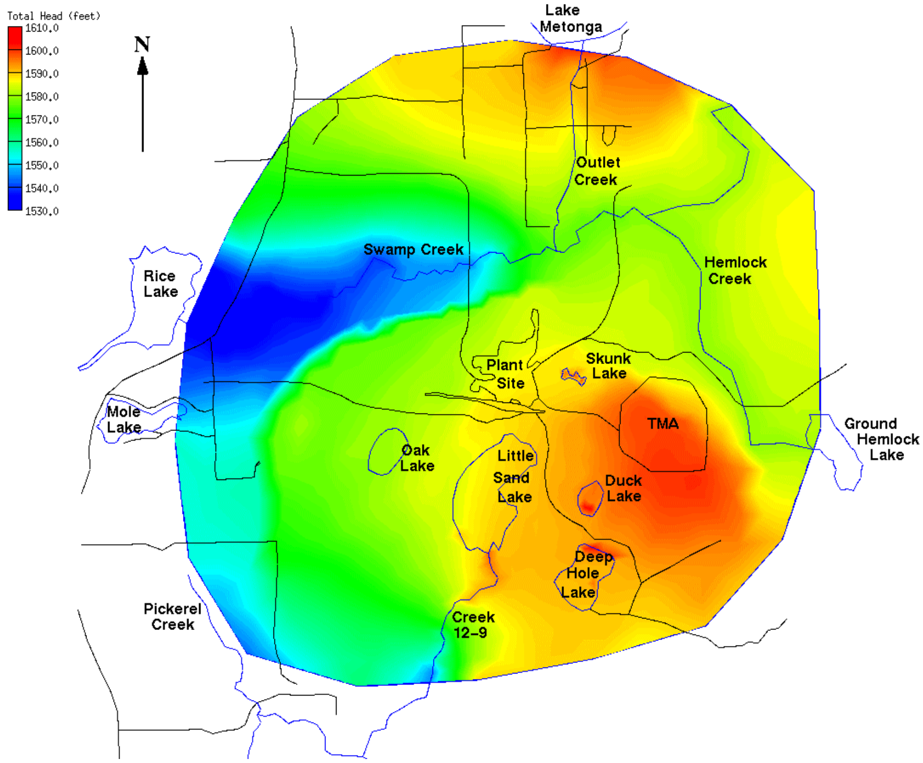

Figure 4. Total head continuous tone contours

Approximate Newton method with dynamic relaxation

The nonlinear Picarde iteration was replaced with an approximate Newton method with dynamic relaxation because the problem would not converge. The system of nonlinear equations

$$[M]^{n+1}\left(\{h\}^{n+1} - \{h\}^{n}\right) + \Delta t[K]^{n+1}\{h\}^{n+1} = \Delta t\{Q\}^{n+1} \tag{1}$$

is linearized to

$$\begin{aligned} &\left([M]^{j} + \Delta t[K]^{j}\right)\{\delta h\}^{j+1} = [M]^{j}\left(\{h\}^{n} - \{h\}^{j}\right) + \Delta t\left(\{Q\}^{j} - [K]^{j}\{h\}^{j}\right) \\ &\{h\}^{j+1} = \{h\}^{j} + f_{\%}\{\delta h\}^{j+1} \end{aligned} \tag{2}$$

where

[M] - mass matrix

[K] - stiffness matrix

{h} - pressure vector

{Q} - external flow vector

{δh} - change in pressure vector

Δt - time increment

j - nonlinear iteration index

n - time step index

$f_{\%}$ - nonlinear relaxation factor, $0 < f_{\%} < 1$

Sometimes the nonlinear solution stalls from $f_{\%}$ being too small, and sometimes it oscillates from $f_{\%}$ being too large. To overcome this situation, we established the following criteria. If the maximum residual for the current iteration is less than the last nonlinear iteration, then set $f_{\%} = f_{\%} + 0.005$ up to a maximum value of 1. If the maximum residual for the current iteration is greater than the last nonlinear iteration, then set $f_{\%} = (2/3)\, f_{\%}$ down to a minimum value of 0.1.

Recursive halving of the time step

There were still some troublesome areas that required further refinement. Therefore, a recursive halving of the time step was implemented. The equations for two halving reductions are as follows:

$$
\begin{aligned}
[M]^{n+\frac{1}{2}}\left(\{h\}^{n+\frac{1}{2}} - \{h\}^{n}\right) + \frac{\Delta t}{2}[K]^{n+\frac{1}{2}}\{h\}^{n+\frac{1}{2}} &= \frac{\Delta t}{2}\{Q\}^{n+1} \\
[M]^{n+\frac{3}{4}}\left(\{h\}^{n+\frac{3}{4}} - \{h\}^{n+\frac{1}{2}}\right) + \frac{\Delta t}{4}[K]^{n+\frac{3}{4}}\{h\}^{n+\frac{3}{4}} &= \frac{\Delta t}{4}\{Q\}^{n+1} \\
[M]^{n+1}\left(\{h\}^{n+1} - \{h\}^{n+\frac{3}{4}}\right) + \frac{\Delta t}{4}[K]^{n+1}\{h\}^{n+1} &= \frac{\Delta t}{4}\{Q\}^{n+1}
\end{aligned}
\qquad (3)
$$

where the right-hand side is unchanged in the current implementation. This allowed the problem to advance over troublesome spots.

Soil property curves

FEMWATER uses soil property curves to model such things as relative hydraulic conductivity versus pressure head in its computation. Sometimes the curves have points concentrated near zero as shown in Figure 5. As FEMWATER uses linear interpolation to navigate along these curves, sometimes the nonlinear iteration hangs up when using tolerances of 10^{-4}. The solution to this problem was to take out points near zero. This does not change the nature of the curve, yet it substantially reduces the convergence time and the need to recursively subdivide the time step.

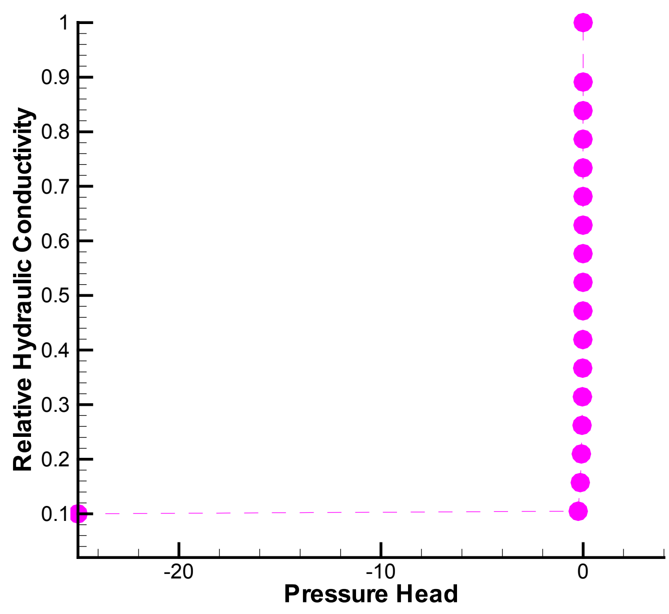

Figure 5. Relative hydraulic conductivity versus pressure head

Solvers

The last issue that helped in reducing the running time and allowed the successful completion of the 29 year study is solvers. As the same phenomena occurred in the military site cleanup problem discussed next, this will be addressed and emphasized in that application.

Remediation Plan for a Large Military Site

Description of the problem

The conceptual model includes facilities from the military base and all surrounding municipal activities that might impact the flow field within the base perimeter. The selected area of the surface model domain approximates the geometry of a trapezoid with east-west dimensions of 6880 and 12440 ft and north-south dimensions of 19440 and 18680 ft. The military site is roughly centered in the trapezoid that includes part of the municipal community. A two-dimensional mesh which includes military base monitor wells and 39 extraction wells, three municipal wells, six pond test locations, and an irrigation ditch was generated by the GMS map module and manually refined around hydrogeologic computational problem areas (Figure 6.). The final two-dimensional mesh included 8583 nodes and 17082 elements. Different numbers of vertical computational layers and pumping and ponding options were then considered using 3-D meshes created from the 2-D mesh and || FEMWATER to help in developing a remediation plan. Figure 7 shows pressure head data, velocity vector data, and plume boundary for a dynamic simulation of a 11-layer flow simulation.

Solvers

A classical stationary symmetric relaxation iterative solver and a conjugate gradient solver were both successfully used to produce results for meshes containing approximately 450,000 3-D elements.

Conjugate gradient solver

Typically, the approach is to solve the linear system of equations such as those given in Equation 2 accurately before going to the next nonlinear iteration. However, it was consistently found that loosening the criteria and not solving the system of linear equations as accurately improved the over-all running time as shown in Table 1. Remarkably, reducing the maximum iterations to 500 not only halved the original running time when 3000 iterations were used initially but also the number of nonlinear iterations was also reduced. It should also be noted that as in the 1000 iteration case, an inefficient set of pe's is obtained, showing inconsistent timings. At 200 iterations the conjugate gradient method would not converge.

Symmetric relaxation iterative solver

This solver first does a relaxation going forward from one to the number of nodes and then backward from the number of nodes to one to become symmetric. The parallel version of this solver is less efficient than the scalar version because it is implemented like a domain decomposition method with specified head given for the pe boundary conditions (see Figure 8). This weakens the convergence of the algorithm such that problems that can use a relaxation factor of 1 (Gauss-Seidel iteration) on a one pe machine sometimes diverge on a parallel

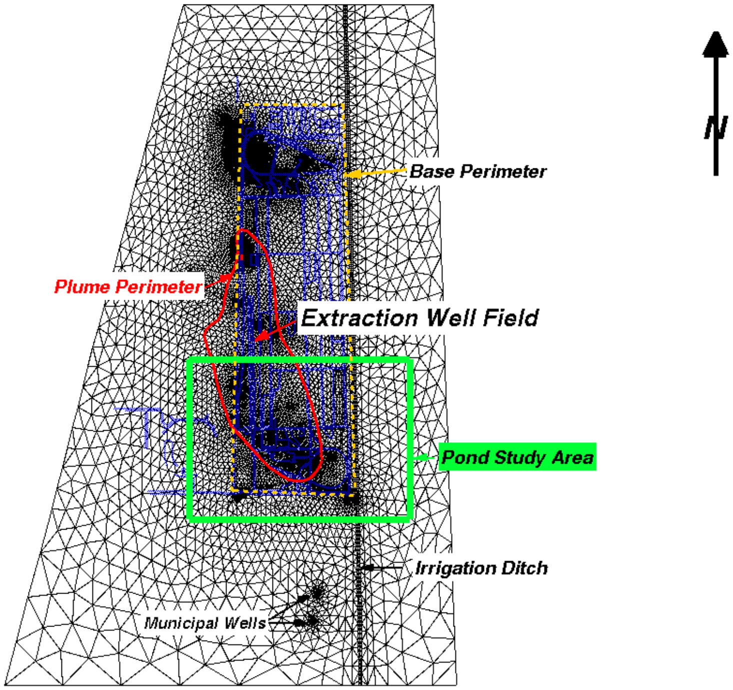

Figure 6. Surface model domain

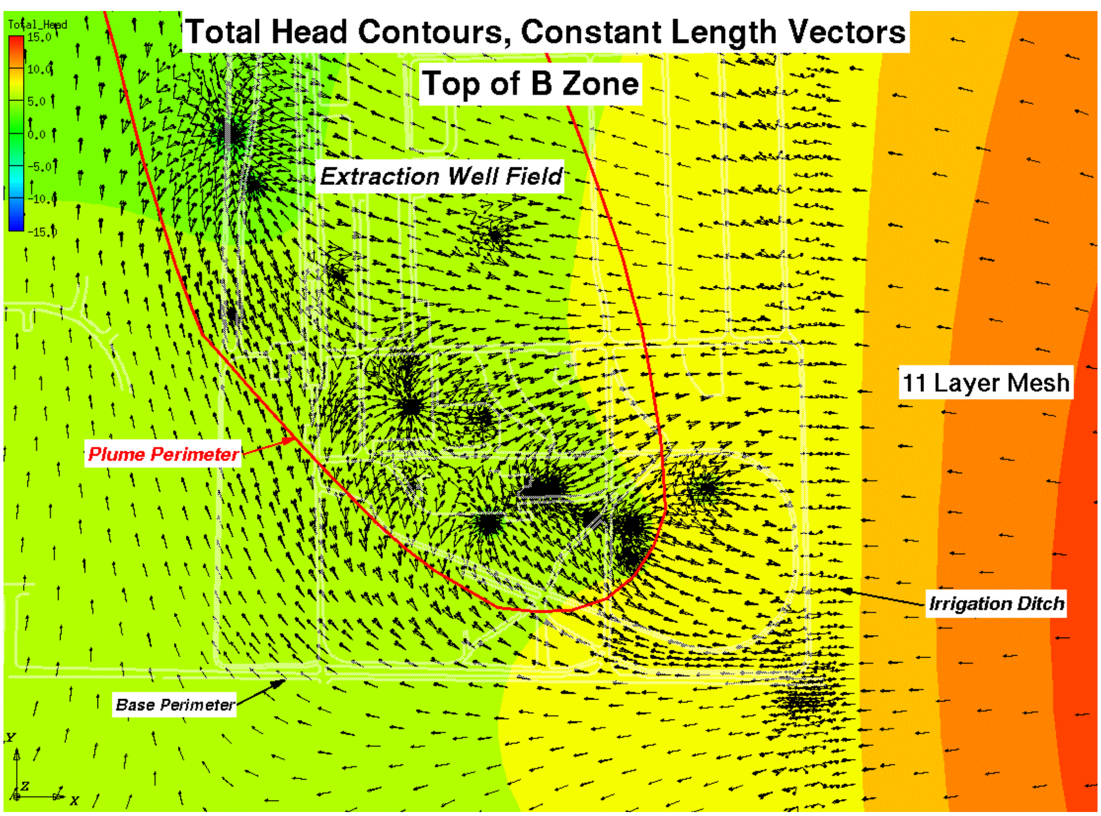

Figure 7. Flow velocities and total head

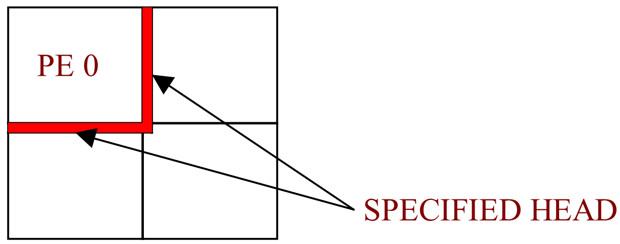

Figure 8. Domain decomposition

computer. Also, the results given in Table 2 do not show the same improvement as the number of linear iterations are decreased as in the case of the conjugate gradient method, although the problem always converges for this steady-state run. Regardless, this solver with the relaxation factor being set to one-half still out-performs the conjugate gradient solver for this particular problem.

Future Plans and Conclusion

More sophisticated solvers that use Krylov methods, multigrid pre-conditioning, GMRES, etc. will be tried for potential improvement. B splines will also be considered for the soil property curves. Also, a new version that includes subsurface, overland flow, and canals is being parallelized. Larger models will also be generated and run. However, the current version of || FEMWATER has been successfully applied to the real-world engineering applications of a deep mine project and the cleanup of a large military site.

References

1. Lin, H.J., Richards, D.R., Talbot, C.A., Yeh, G.T., Cheng, J.R., Cheng, H.P., and Jones, N.L., FEMWATER: A Three-Dimensional Finite Element Computer Model for Simulating Density-Dependent Flow and Transport in Variably Saturated Media, Technical Report CHL-97-12, U.S. Army Engineer Waterways Experiment Station, MS, July 1997.

2. Groundwater Modeling Team, *GMS*, http://chl.wes.army.mil/software/gms/, U.S. Army Engineer Waterways Experiment Station, MS.

3. Karypis, G., *METIS*, http://www-users.cs.umn.edu/~karypis/metis/metis.html, University of Minnesota, MN.

Figures

Tables

Maximum linear iterations	Nonlinear iterations	Time (sec)
3000	55	690.7
2000	55	630.5
1000	55	742.6
500	37	375.6
200	~	~

Table 1. Conjugate gradient solver results

Maximum linear iterations	Nonlinear iterations	Time (sec)
1000	25	243.7
500	21	228.3
200	38	252.1
100	89	317.9
50	287	652.8
20	1024	1351.5

Table 2. Symmetric relaxation solver results