AIM

Association for Information and Image Management

1100 Wayne Avenue, Suite 1100
Silver Spring, Maryland 20910
301/587-8202

Centimeter

Inches

MANUFACTURED TO AIM STANDARDS
BY APPLIED IMAGE, INC.

1 of 1

UCRL-JC-115374
PREPRINT

Use of High Performance Computing to Examine the Effectiveness of Aquifer Remediation

A.F.B. Tompson
S.F. Ashby
R.D. Falgout
S.G. Smith
T.W. Fogwell
G.A. Loosmore

This paper was prepared for submittal to the
X International Conference on Computational
Methods in Water Resources
Heidelberg, Germany
July 19-22, 1994

June 1994

RECEIVED

APR 04 1994

OSTI

MASTER

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

DISCLAIMER

This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor the University of California nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial products, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or the University of California, and shall not be used for advertising or product endorsement purposes.

USE OF HIGH PERFORMANCE COMPUTING TO EXAMINE THE EFFECTIVENESS OF AQUIFER REMEDIATION

A. F. B. TOMPSON¹, S. F. ASHBY², R. D. FALGOUT², S. G. SMITH², T. W. FOGWELL³, and G. A. LOOSMORE⁴

¹Earth Sciences Division, L-206; ²Computing and Mathematics Research Division, L-316, Lawrence Livermore National Laboratory, University of California, PO Box 808, Livermore, CA 94551, USA

³IT Corporation, Martinez, CA 94553, USA

⁴Department of Applied Science, University of California-Davis, Livermore, CA 94550, USA

Large-scale simulation of fluid flow and chemical migration is being used to study the effectiveness of pump-and-treat restoration of a contaminated, saturated aquifer. A three-element approach focusing on geostatistical representations of heterogeneous aquifers, high-performance computing strategies for simulating flow, migration, and reaction processes in large three-dimensional systems, and highly-resolved simulations of flow and chemical migration in porous formations will be discussed. Results from a preliminary application of this approach to examine pumping behavior at a real, heterogeneous field site will be presented. Future activities will emphasize parallel computations in larger, dynamic, and nonlinear (two-phase) flow problems as well as improved interpretive methods for defining detailed material property distributions.

INTRODUCTION

Predictive modeling of fluid flow, chemical migration, and transformation processes in the subsurface is widely applied within the oil industry and in the management of environmental contamination problems [8]. Computational models are routinely used to characterize gross rates of groundwater flow, contaminant migration and chemical transformation in the subsurface, design, analyze, or optimize the performance of remediation projects, estimate associated health risks, or demonstrate compliance with federal and state cleanup regulations.

In subsurface contamination problems, the porous soil environments are typically large (0.1-10km), complex, and nonuniform, and differ from the smaller (1m), idealized, and controlled laboratory systems where flow and transport phenomena in porous media are typically studied. This had led to increasing concern about the influence of aquifer heterogeneity on flow, transport, and remediation processes and how they are represented in field modeling applications [4,6]. Uncertainty and complexity in flow or transport behavior can be produced by small-scale (1m) variability in formation materials and their associated properties, constraints on the type and quantity of measurements available to characterize real systems, or oversimplified representations of the fundamental processes present. Failure to recognize or incorporate the effects of small-scale process interactions in field scale models could ultimately lead to unreliable conclusions about system behavior.

Figure 1: Perspective conceptualization of the upper aquifer beneath LLNL showing alluvial materials (white), less permeable uplifted zones (dark), a nearby fault zone, and the sample volume used for detailed simulation.

Hence, we are developing and applying highly-resolved computational models of flow, migration, and transformation phenomena to study the impacts of medium heterogeneity on aquifer-scale behavior and remediation efficiency. As a complement to theoretical and experimental analysis, detailed calculations have been used to validate the accuracy of scaling or homogenization theories, benchmark the performance of intermediate or field scale experiments, or test and simulate the efficacy of specific remediation schemes within nonuniform environments [1,7,9,10,14,15]. Modeling capabilities that address behavior in three dimensions, resolve important small-scale property variations, and incorporate specific remediation technologies or processes are typically required. Such problems may have upwards of 10^9 nodes and may require solution approaches on massively parallel computers [3,5].

EXAMPLE FIELD APPLICATION

As an example application, we consider the groundwater flow and chemical migration processes in the upper alluvial materials beneath the Lawrence Livermore National Laboratory (LLNL) in California. The groundwater in this area was contaminated with some 8 volatile organic compounds (VOC) 50 years ago when the lab site was occupied by a naval airfield. The existing saturated zone contamination extends from beneath LLNL to over a mile west, is slowly moving toward municipal wells in downtown Livermore, and is the focus of a large pump-and-treat remediation project [12]. In Figure 1, a schematic of the upper aquifer beneath LLNL shows the alluvial materials, several less permeable uplifted zones, a nearby fault zone, and the location of the downtown wells. The lower boundary of the aquifer overlays a relatively consistent, impermeable blue clay formation throughout the region. Flow in the alluvium goes mainly from the east and southeast toward the west.

Several 2-D modeling studies of flow and transport in the regional LLNL system have been carried out, under both natural and remedial conditions [17,18]. These have been based on simplified, or “effective” representations of flow and transport processes, a small

number of physical and chemical property measurements, a reasonable amount of geologic interpretation, and some limited application of stochastic flow theory [16]. We seek here to develop a more focused 3-D modeling study in which the basic material heterogeneities are resolved and their subsequent impacts on flow and transport can be more carefully approximated. In this sense, uncertainties about the representation of effective behavior can be reduced by increasing the computational effort and property resolution.

SIMULATION APPROACH

Simulation Domain. For simplicity, our initial study volume is comprised of a 12,700 ft square prismatic block of alluvium “carved” out of the upper 320 feet of saturated aquifer surrounding the LLNL site (Figure 1). The origin of a coordinate system with $+x$ to the east, $+y$ to the north, and $+z$ up is at the lower southwest corner. The lower portion of the block intersects the bounding clay formation, while its southeast corner is crossed by the fault zone. The upper portion corresponds to the water table. Material properties such as the hydraulic conductivity, medium porosity, or mineral sorptive capacity will be specified separately for the alluvial materials, the lower clay layer, and the fault zone. As motivated by interpretive arguments below, we have chosen a rather coarse discretization involving $128 \times 128 \times 64$ (or over 10^6) nodes for this initial study, where $\Delta x = \Delta y = 100$ ft, and $\Delta z = 5$ ft.

Balance Laws. Steady, saturated flow in this system is described by [4]

$$\epsilon \mathbf{v} = -K \nabla h, \quad (1)$$

where $\mathbf{v}(\mathbf{x})$ is the average groundwater seepage velocity [L/T], $h(\mathbf{x})$ is the hydraulic head [L], K is the medium hydraulic conductivity, and ϵ is the medium porosity. In saturated and nondeforming media, h satisfies

$$\nabla \cdot (K \nabla h) = -Q, \quad (2)$$

where $Q > 0$ [1/T] represents a loss of fluid due to pumping. Physical medium heterogeneities may be reflected in spatially dependent values of K or ϵ .

The migration of one or more dissolved, sorbing, and neutrally-buoyant chemicals in the groundwater is described by [15]

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot \left(\frac{\mathbf{v} \rho_i}{\mathcal{R}_i} \right) - \nabla \cdot \left(\epsilon \mathbf{D}_i \cdot \nabla \left(\frac{\rho_i}{\epsilon \mathcal{R}_i} \right) \right) = - \left(\frac{\rho_i}{\epsilon \mathcal{R}_i} \right) Q \quad (3)$$

where $\rho_i(\mathbf{x}, t)$ is the total (liquid + sorbed) concentration [M/L³] of chemical i at a point in the medium. The quantity $\mathbf{D}_i \approx \alpha_T |\mathbf{v}| \mathbf{I} + (\alpha_L - \alpha_T) \mathbf{v} \mathbf{v} / |\mathbf{v}|$ is the velocity-dependent hydrodynamic dispersion tensor [L²/T], and α_L and α_T are the local longitudinal and transverse dispersivities [L]. In (3), we have assumed that sorption onto the mineral phase occurs reversibly and in an equilibrium fashion such that the aqueous concentration (c_i) may be inverted from $\rho_i = \epsilon c_i \mathcal{R}_i$. Here, the quantity $\mathcal{R}_i$ represents the local partitioning or retardation capacity of the soil, and may generally be concentration dependent. In the experiments below, we consider a nonreactive tracer ($i = 1$) and a linearly sorbing compound ($i = 2$) such that $\mathcal{R}_1 = 1$ and $\mathcal{R}_2 = 1 + \epsilon k_d / (1 - \epsilon)$, where k_d is a dimensionless sorption

coefficient. In this case, medium heterogeneity may be reflected in spatially dependent values of α_L , α_T , or k_d .

Specification of Material Properties. Because we cannot specify detailed property distributions from measurement alone, simulations will be made in one or more realizations of the system that preserve or recreate estimated statistical patterns of heterogeneity in the alluvium, while retaining the larger clay and fault zones as bulk features with constant properties. In the alluvium, heterogeneity in the hydraulic conductivity (K) will be developed from an approximate spectral (random field) model [4,13]. Assuming $\ln K(\mathbf{x}) = F + f(\mathbf{x})$, preliminary analyses of site data indicate that the geometric mean conductivity $K_G = e^F \approx 4.0$ ft/day, log- K variance $\sigma_f^2 \approx 3.2$, and exponential model correlation scales $\lambda_i \approx (200, 200, 10)$ ft, respectively [16], leading to the coarse discretization above. Although this is a common and simple model of heterogeneity, alternative representations are also being pursued. In the lower clay and fault materials, K will be assigned constant values of 0.004 and 0.4 ft/day, respectively. The soil sorptivity will be specified from a direct correlation with conductivity through $\ln \epsilon k_d \approx -0.86 - 0.32 \ln K$ [15]. The quantities ϵ , α_L , and α_T will be held constant and set to representative local values of 0.3, 1.0 ft, and 0.1 ft, respectively.

Solution of Equations. Solutions of (2) were determined in the study volume using a 7-point finite difference spatial discretization; velocity fields were then derived from (1). Inversion of the 10^6 finite difference equations was performed with a parallel preconditioned conjugate gradient (PCG) technique implemented within the PARFLOW code [2]. Current results are based on 2-step Jacobi preconditioning. In the future, we will employ polynomial and multigrid preconditioners. PARFLOW is being implemented on several distributed memory MIMD machines with message passing, including the nCUBE/2, Cray T3D, and Meiko CS-2, as well as on workstation clusters. The code achieves portability by using a communications layer called AMPS, which is ported on top of either PVM [3], the REACTIVE KERNEL/COSMIC ENVIRONMENT [11], or vendor message passing primitives. The main source code (written in C) is completely portable. The problem data is distributed onto a logical process mesh; physical mappings are handled by AMPS. Specifically, we distribute the unknown pressure heads and the underlying 7-point PDE stencil across the processes, along with auxiliary data. Realizations of the random hydraulic conductivity distribution are generated dynamically within PARFLOW using a parallel, C version of the turning bands TURN3D code [13]. This avoids input/output bottlenecks when full sets of parametric data are distributed from disk to the processors. Smaller sets of data representing fault or clay zone properties are read in from disk following the spectral generation. Once initialized, steady head solutions for our study volume were generated using 864 dedicated nodes of an nCUBE/2. The solution of a single problem with 10^6 mesh points required approximately 3500 PCG iterations and 7.5 minutes of wall-clock CPU. Since PARFLOW demonstrates good scalability (that is, solution times remain constant as larger problems are mapped onto larger processor arrays), the resolution of our study volume is limited only by the size of the parallel machine.

Solutions of (3) were determined with a serial version of the particle-grid code SLIM, modified to account for mass capture by pumping wells [15]. In this model, the distribution of total mass is distributed among a number of particles that are allowed to move through the flow field in small time increments in response to advective, diffusive, and retardation forces. When extraction wells are present, particles are removed from pre-defined capture

zones as a function of the time step and retardation strength. The particle-grid algorithm is well suited for efficient solution of transport problems involving small point sources of mass in large, highly resolved flow domains.

SOME RESULTS

Realization #1 of the conductivity distribution for the study volume is shown in Figure 2a. The orientation is similar to the cut-out location indicated in Figure 1. In Figure 2, a block of the volume has been removed to show the internal structure, including the fault and lower clay zones. Two separate flow solutions were obtained for this problem. Solution "1a" corresponds to ambient conditions, with no-flux (or confined) conditions enforced at the top and bottom, and specified heads along the four sides. The head values were interpolated from regional measurements of the piezometric surface and were assumed constant over depth. Solution "1b" includes a pumping well at node (65,65,33), close to the center of the volume. This was specified by maintaining a fixed head value of 530 ft at the node. The resulting extraction rate was determined from a mass balance to be 24,000 ft³/day, or 0.28 ft³/sec. The head and velocity magnitude distributions for solution 1b are also shown in Figure 2, the effect of the well being marginally detectable near the corner of the cut-out block. Four other pairs of flow realizations (not shown) were developed in the same way. A sixth pair of flow fields (not shown) were developed by setting the alluvial conductivity uniformly equal to the geometric mean conductivity, $K_G = 4.0$ ft/day. Figure

Figure 2: Distribution of hydraulic conductivity, head, and velocity magnitude for problem 1b

3a shows averages of the velocity components (and velocity magnitude) in the alluvium for

solution 1a. These were determined in a $4\Delta x$ -wide y-z slab of the block, as a function of its location on the x-axis. Similar results averaged over all 5 “a” runs do not show much difference. Groundwater generally moves toward the northwest, albeit faster in the western locations where there is a converging flow effect. In Figure 3b, the variance of the velocity components (and their magnitude) as determined in the same moving slab are shown for the single run 1a and ensemble “a” runs. Here, the trend is for larger variances in the west where the mean velocities are larger as well. The high values at either end are an artifact of the fixed boundary conditions. Several transport problems were developed that focused

Figure 3: “y-z” averages and variances of the alluvium velocity components, as a function of the x-coordinate; thin lines = problem 1a, thick lines = ensemble over 5 replicate “a” runs.

on the migration of small pulses of the tracer and reactive compounds placed near node (95,30,45), in the southeast part of the block, to the north of the fault zone. Roughly 6.8 kg (liquid) and 10.2 kg (liquid + sorbed) of components 1 and 2 were released into the system, both corresponding to 1 ppm initial aqueous concentrations. Different flow field pairs were used to evolve different migration scenarios. Particles representing both compounds were released in the ambient “a” fields for 20000 days (55 yr), after which the central extraction well was turned and the corresponding “b” fields were used. Mass migration and capture were monitored for the next 30000 days, to 137 years after the initial release.

In Figure 4a, the average x-y mass distribution derived with flow solution 1a is shown for both components in a bird’s eye perspective at $t = 20000$ days (closed circles represent the nonreacting tracer). Portions of both components have moved past the well by this time. Figure 1b shows the mass recovered after the well has been turned on, as a function of time (solid lines represent the nonreacting tracer). Recovery curves obtained with the 4 other pairs of flow flow realizations are also shown. In general, recovery of the reactive mass (1020 kg) takes longer, but is more complete because of the timing of turning the well on. Differences in the results arise from the separate property realizations, most importantly from their local effect on the initial mass distributions.

In Figure 4b, the same set of figures is shown for the case where flow solution 6 (based upon a uniform alluvial conductivity of K_G) is used. Here we see no macrodispersion arising from heterogeneity. We also see a slower effective plume velocity, caused because the “effective” conductivity of the heterogeneous system in problem 1 should be greater

than K_G [1,6,16]. No recovery of component 2 is found.

In Figure 4c, the problem in flow field 6 is run again, except that the values of α_L and α_T in the transport model are increased to 265.0 and 26.5 ft., respectively, to approximate their macroscopic counterparts estimated from stochastic theory [16]. Here we see more significant spreading, some of which moves upstream of the source. Although the ratio α_L/α_T is too small, the longitudinal value may actually reproduce the effects in Fig. 4a if a more reasonable effective velocity is used. Mass recovery is poor because the excessive transverse spreading moves mass outside the capture zone of the well.

Figure 4: Particle and recovery plots (see text)

Acknowledgements. This work was conducted under the auspices of the U. S. Department of Energy by Lawrence Livermore National Laboratory under contract W-7405-Eng-48. It was supported, in part, by the Laboratory Directed Research and Development program and the Strategic Environmental Research and Development Program of the U. S. Department of Defense, through the cooperation of the USAE Waterways Experiment Station, Vicksburg, MS.

REFERENCES

- 1 Ababou, R., D. B. McLaughlin, L. W. Gelhar, Three-Dimensional Flow in Random Porous Media, Massachusetts Institute of Technology (R. M. Parsons Laboratory Report #318), 1988.
- 2 Ashby, S. F., R. D. Falgout, S. G. Smith, and A. F. B. Thompson, *Modeling Groundwater Flow on MPPs*, Proc. 1993 Scalable Parallel Libraries Conference, October 6-8, 1993, Mississippi State University; also Lawrence Livermore National Laboratory, Livermore CA (UCRL-JC 115602), 1993
- 3 Beguelin, A., J. Dongarra, G. A. Geist, R. Manchek, and V. Sunderam, *A users' guide to PVM: Parallel Virtual Machine*, Oak Ridge National Laboratory (ORNL/TM-11826), July, 1991.
- 4 Dagan, G., *Flow and Transport in Porous Formations*, Springer Verlag, 1989
- 5 Dougherty, D. E., *Hydrologic Applications of the Connection Machine CM-2*, Wat. Resour. Res., 27, pp 3137-3147, 1991
- 6 Gelhar, L. W., *Stochastic subsurface hydrology: from theory to applications*, Water Resources Res., 22(9), p 135s, 1986
- 7 Kinzelbach, W., *The random walk method in pollutant transport simulation*, in Groundwater Flow and Quality Modelling, E. Custodio, A. Gurgui, and J. P. Lobo Ferreira, eds., D. Riedel, Dordrecht, The Netherlands, pp 227-246, 1987
- 8 National Research Council, Ground water models: Scientific and Regulatory Applications, National Academy Press, Washington, 1990
- 9 Polmann, D., McLaughlin, D., S. Luis, L. Gelhar, and R. Ababou, *Stochastic modeling of large scale flow in heterogeneous, unsaturated soils*, Water Resources Res., 27(7), 1447-1458, 1991
- 10 Schäfer, W. and W. Kinzelbach, *Stochastic modeling of in-situ bioremediation in heterogeneous aquifers*, J. Contam. Hydrol. 10, pp 47-73, 1992
- 11 Seitz, C. L., J. Seizovic, and W.-K. Su, *The C Programmer's Abbreviated Guide to Multicomputer Programming*, California Institute of Technology, (Caltech-CS-TR-88-1), January, 1988.
- 12 Thorpe, R. K., W. F. Isherwood, M. D. Dresen, and C. P. Webster-Scholten, Eds., *CERCLA Remedial Investigations Report for the LLNL Livermore Site*, Lawrence Livermore National Laboratory, Livermore, CA (UCAR-10299), 1990.
- 13 Thompson, A. F. B., R. Ababou, and L. W. Gelhar, *Implementation of the three-dimensional turning bands random field generator*, Wat. Resour. Res., 25(10), pp 2227-2243, 1989
- 14 Thompson, A. F. B. and L. W. Gelhar, *Numerical simulation of solute transport in randomly heterogeneous porous media*, Wat. Resour. Res., 26, pp 2541-2562, 1990
- 15 Thompson, A. F. B., *Numerical simulation of chemical migration in physically and chemically heterogeneous porous media*, Wat. Resour. Res., 29, pp3709-3726, 1993.
- 16 Thompson, A. F. B., *Flow and Transport within the Saturated Zone Beneath Lawrence Livermore National Laboratory: Modeling Considerations for Heterogeneous Media*, Lawrence Livermore National Laboratory, Livermore CA (UCID 21828), 1990.
- 17 Thompson, A. F. B., E. M. Nichols, P. F. McKereghan, and M. C. Small, *Summary of Preliminary Ground Water Simulations in the Livermore Regional Modeling Study - CFEST Finite Element Code*, Lawrence Livermore National Laboratory, (UCRL-AR-107049), 1991.
- 18 Thompson, A. F. B., E. M. Nichols, and P. F. McKereghan, Eds., *Preliminary Simulation of Contaminant Migration at the Lawrence Livermore National Laboratory*, Lawrence Livermore National Laboratory, (UCRL-AR-report in preparation), 1994.

DATE

FILMED

6 / 30 / 94

END