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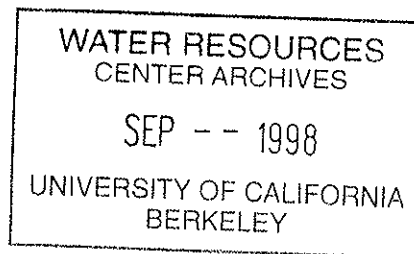
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# ADAPTIVE GRID REFINEMENT FOR GROUNDWATER CONTAMINANT TRANSPORT SIMULATION

## *TECHNICAL COMPLETION REPORT*



California Water Resources Center Project W-737

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# ADAPTIVE GRID REFINEMENT FOR GROUNDWATER CONTAMINANT TRANSPORT SIMULATION

## ABSTRACT

Mathematical models of the transport and fate of dissolved chemicals in groundwater are becoming increasingly important tools in understanding, managing, and remediating groundwater contamination. The success of such models is dependent on: 1) how well the relevant physical, chemical, and microbiological processes controlling subsurface transport are represented with mathematical equations, and 2) how accurately and efficiently the equations are solved with numerical methods that discretize the equations over space and time. The computational burden associated with multidimensional, multicomponent, numerical solute transport models can be prohibitive. In this project, we have implemented and extended a local adaptive grid refinement (LAGR) method of Berger and Olinger (1984) to solve CPU-intensive transport problems efficiently and accurately. The method tracks error-prone regions of the solution domain and supplies high-resolution subgrids where they are locally needed while maintaining relatively few nodes elsewhere on a coarse base grid. Novel features include a unique method for detecting a priori where the numerical error is unacceptable, variable time step control which allows smaller time steps on subgrids than on the base grid, and a modular framework which allows easy exchange of partial differential equation solvers to accommodate different problem formulations.

We use simulations for uniform and nonuniform flow fields and for single, nonreactive species and multiple, reactive species to demonstrate and evaluate the LAGR method. The cost and accuracy of LAGR simulations depends on design parameters controlling where subgrids are created, how frequently they are created, and how large they are once they are created. For any particular problem there is a trade-off between cost and accuracy, depending on how the design parameters are chosen. Although the optimal set of design parameters is nonunique, we have been able to provide important insight into the choice of parameters for a desired solution accuracy. Using this insight, solutions with accuracies comparable to those achieved with a uniform fine grid are obtained at between 15 and 30% of the computational cost.

## INTRODUCTION

Contamination of groundwater resources by toxic and hazardous chemical has become a matter of increasing concern in recent years. Proper management of groundwater quality requires expedient policy and efficient corrective action design when necessary. Rarely are either of these implemented without debate or trade-offs. Improving our understanding of the movement, fate, and effect of subsurface contaminants reduces the uncertainty associated with such decisions and, therefore, leads to more efficient resource management.

Studies aimed at understanding, managing, and remediating groundwater contamination are increasingly using numerical solutions of mathematical models describing the transport and fate of dissolved chemicals. Numerical methods are necessary when model complexity exceeds the capability of standard analytical techniques, e.g., when spatially varying parameters and coupled nonlinear equations are involved. Rapid advances in solution methodologies and computer hardware have pushed the frontier of such models to larger and more complicated problem formulations. However, there remains a need for more efficient algorithms. Proper design and analysis studies require repeated calculations to evaluate uncertainty in the parameter space. The desire to assess increasingly complex physical, chemical, and microbiological processes in two- and three-dimensional model formulations continues to challenge our computational abilities.

Even for simple mathematical descriptions of solute transport processes, such as the advection and dispersion of a single, non-reacting species, accurately approximating solutions of the governing equations with numerical methods can be a difficult task. Experience demonstrates that contaminant concentrations may change orders of magnitude over very short distances. However, such concentration fronts often occupy only a small portion of the computational domain at any instant in time. Many traditional solution techniques require a fine mesh over the entire domain in order to resolve these fine, propagating local structure without incurring undesirable numerical errors such as oscillations and numerical dispersion. Because high resolution is not needed in portions of the domain where the solution has moderate, rather than sharp, variation, uniform fine discretization is inefficient. For some problems, this inefficiency can be tolerated. For others it can be prohibitively expensive in terms of computational memory requirements or simulation times. Thus, such problems are well-suited for adaptive numerical methods which seek to determine a priori where increased numerical resolution is required and then provide the necessary high numerical resolution in these regions while providing adequate coarser resolution elsewhere.

## PROJECT OBJECTIVES

The objective of this project is to implement, extend, and evaluate a local adaptive grid refinement (LAGR) method for efficient and accurate numerical solutions to hyperbolic partial differential equations due to Berger and Olinger (1984). The goal is to extend this approach to problems of groundwater transport in complex geological and geochemical environments.

The specific objectives focus on applying LAGR to a set of successively more complex transport problems, beginning with non-reactive transport in a uniform flow field and proceeding to reactive, multi-component transport in a nonuniform flow field. These test problems aim to: 1) evaluate the degree to which LAGR yields better results than those obtained on a uniformly discretized grid; 2) demonstrate that LAGR is a general purpose tool easily amenable to changes in the specific solver and hence the problem formulation; and 3) evaluate the cost and accuracy of the LAGR simulations as functions of the user-specified design parameters. The third objective involves evaluation of methods for choosing the design parameters prior to simulation.

## METHODS

We focus on the partial differential equations describing the mass balance of dissolved species being transported in groundwater under the influence of advection, conventional dispersion, and homogeneous and heterogeneous, instantaneous, chemical reactions, i.e., local chemical equilibrium. The resulting coupled, mixed hyperbolic-parabolic differential equations with auxiliary nonlinear algebraic equations are formulated using Rubin's (1983, 1990, 1991) feed forward method. For convenience alone, we restrict our attention to two-dimensional flow fields.

LAGR achieves accuracy efficiently by automatically creating high-resolution patch grids in regions of the computational domain estimated to have high numerical error, such as at concentration fronts. These patch grids are created and destroyed as these regions move during the simulation. The solver for all grids is the same and integrates the governing equations over a uniformly discretized, rectangular grid.

The basic form of the LAGR method was first presented by Berger and Olinger (1984) for simulation of hyperbolic PDEs. In this project we have adapted it to the coupled, mixed hyperbolic-parabolic PDEs describing reactive groundwater transport, and we have implemented a greatly enhanced modularity so that the method operates independently of the specific solver.

The LAGR algorithm proceeds during one step of integration on a coarse base grid through five steps: 1) truncation error estimation, 2) node flagging and subgrid generation, 3) interpolation of initial and boundary conditions on subgrids, 4) integration through multiple steps on subgrids, and 5) updating coarse grid solution. Initially, the local truncation errors on the base grid are estimated using a Richardson-type extrapolation (Berger and Olinger, 1984). Then, nodes for which the estimated truncation error exceeds a specified tolerance are flagged. The LAGR method proceeds by automatically and efficiently fitting the regions containing flagged nodes with subgrids having finer space and time discretization using nearest neighbor clustering and pattern recognition edge algorithms. Subgrid boundaries are expanded outward to create a buffer zone between the region of high error and the boundary of the new subgrid. Initial and boundary values are linearly interpolated from the coarse grid or from existing fine grids onto the new subgrids. Each subgrid and the base grid are then integrated independently forward in time to the next coarse grid time step where the coarse grid solution is updated with the more accurate subgrid solutions. More detail on each of the steps in the LAGR algorithm is available in Wolfsberg (1993) and Wolfsberg and Freyberg (1994).

For the examples described below computations were performed using a second-order central finite difference spatial discretization and a second-order Runge-Kutta time stepping scheme. We use this explicit method because it parallelizes easily for the IRIS 4D/380GTX Power Series computer. The speed gained through parallel computations outweighs the time step limitation required of this method for stability. However, any finite difference method using a uniform discretization and of the same order in space and time can be couple with the LAGR routines.

Three examples of increasing complexity are briefly described here to demonstrate the implementation and performance of LAGR. We first present solutions to a simple test problem for the single-species, nonreactive, advective-dispersive transport. Next we examine single-species transport in a nonuniform flow field to demonstrate how LAGR creates multiple subgrids to fit complex plume shapes. Finally, we present results for a transport problem involving multiple reactive species.

Figure 1 compares solutions for advective-dispersive transport of an initially Gaussian pulse of a nonreactive species in a uniform velocity field oriented diagonally to the computational grid. For this simple problem an analytic solution is known, and it is shown for an elapsed time of 150 days in Fig. 1(a). Figs. 1(b) and 1(c) show computed finite difference solutions using a uniform fine grid and a uniform coarse grid, respectively. The coarse grid computations clearly lead to oscillations and artificial transverse dispersion creating a "wake" behind the plume. Using LAGR,

with the base grid equivalent to the coarse grid of Fig. 1(c), a refined grid equivalent to that of Fig. 1(b), a buffer zone of two coarse grid blocks, and a regridding interval of four coarse time steps, LAGR achieves the solution shown in Fig. 1(d). The positions of the subgrid at four times are shown in Figure 2. The LAGR solution differs very little from the uniform fine grid solution, and both solutions match the analytical solution well. The LAGR cost, however, is only 18% of the uniform fine grid cost. The size of the subgrid at any time step is between 15% and 20% of the total domain size. Thus, the cost improvement is approximately equal to the ratio of refined region to total computational area.

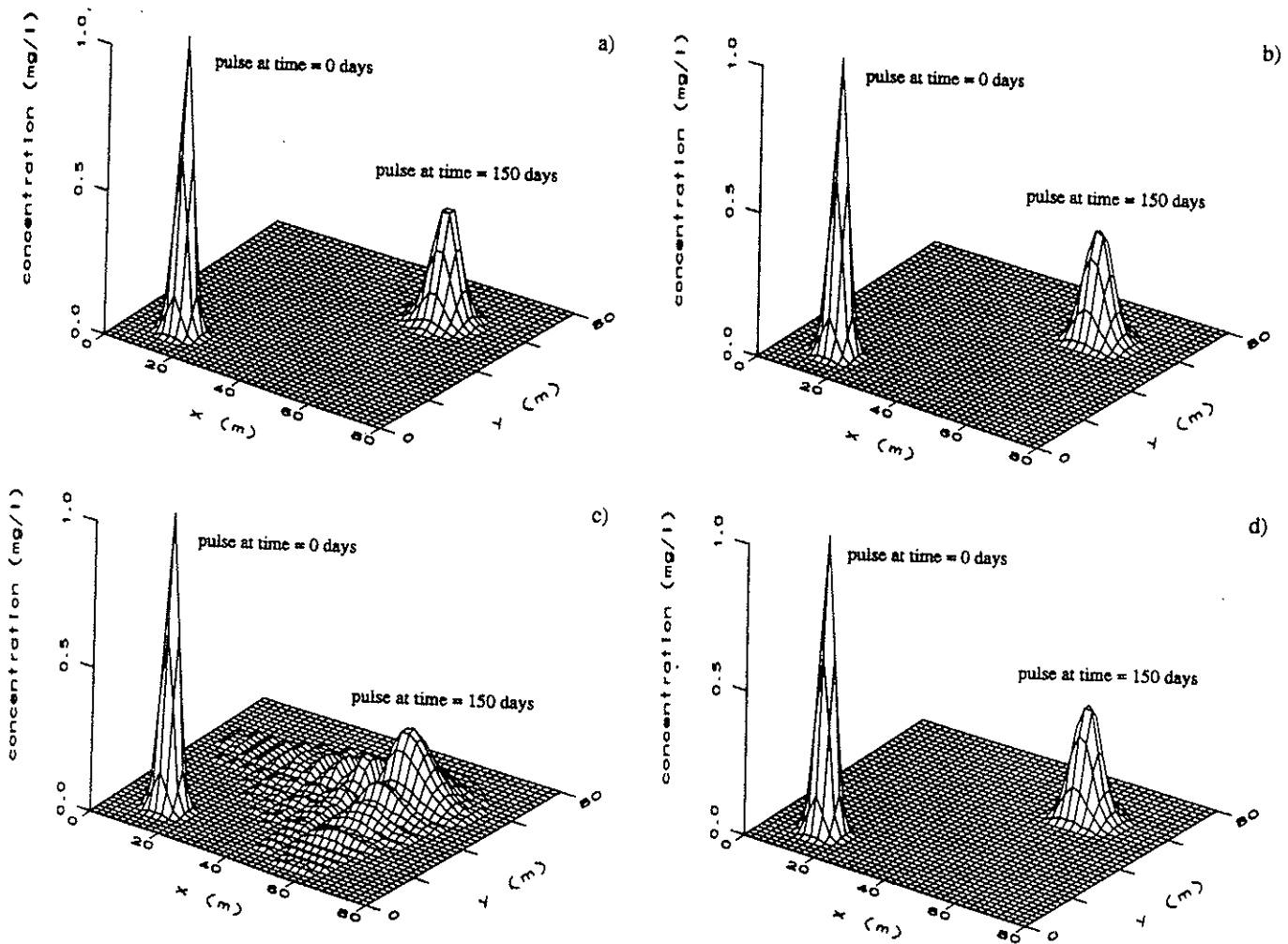


Figure 1. Comparison of solutions for first example problem at an elapsed time of 150 days. (a) Analytical solution. (b) Uniform fine grid. (c) Uniform coarse grid. (d) LAGR. Fine grid is 4X finer than coarse grid in both space and time. All results shown at coarse grid discretization.

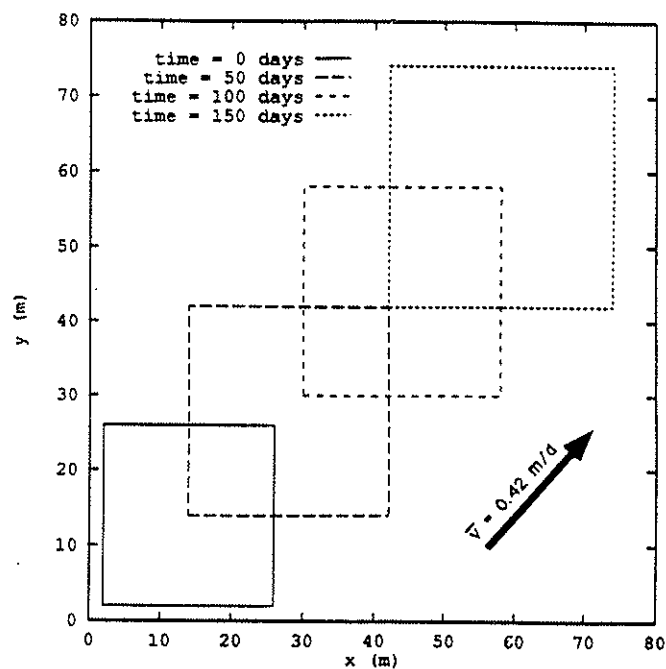


Figure 2. Subgrid placement at elapsed time of 0, 50, 100, and 150 days for the first example problem.

Figure 3 shows the velocity field, in the form of path lines, used for the second illustrative example. The mean seepage velocity in the x direction is 0.12 m/d, while in the y direction it is 0.0 m/d. A constant concentration strip source is centered on the upstream ( $x=0$ ) boundary. Its length is equal to half the width of the domain. The strength of the source remains constant at 1.0 mg/L.

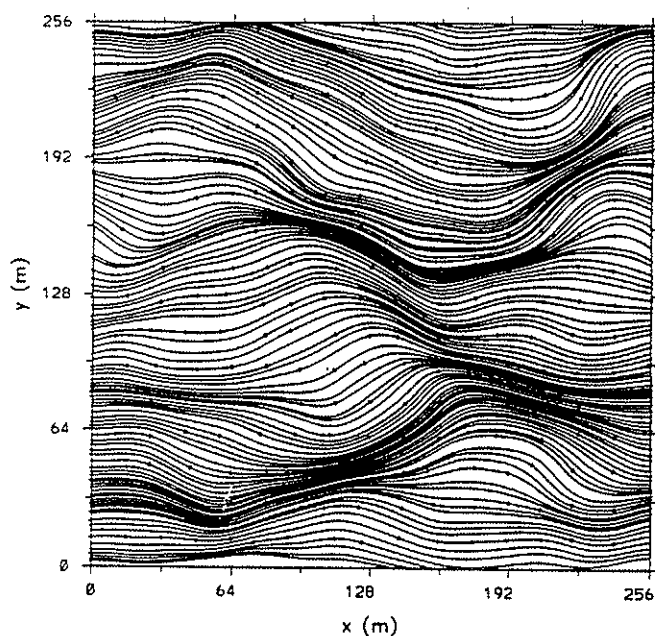


Figure 3. Plan view of flow field path lines for the second illustrative example.

Figure 4 shows the plume after 1000 days, as simulated with a uniform fine grid of 1.0 m squares.

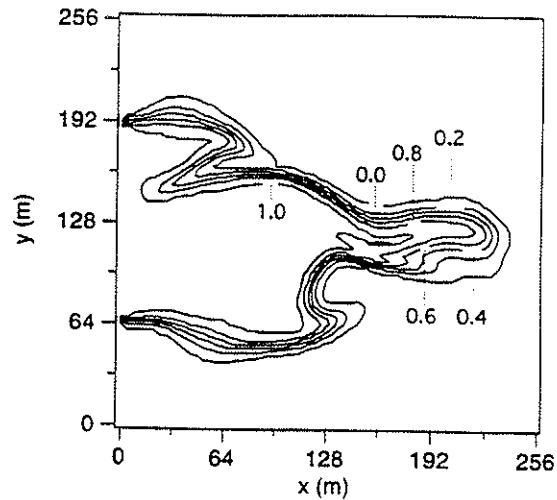


Figure 4. Concentration contours at elapsed time of 1000 days in the second example computed using a uniform fine grid. Concentrations in mg/L.

Figure 5 shows the solution error relative to the uniform fine grid solution using a uniform coarse grid of 4.0 m squares. Recalling that the maximum concentration is 1.0 mg/L, the coarse grid solution is seen to be in error by as much as nearly 40% of the maximum concentration. Large errors are observed near steep concentration gradients along the edges of the plume.

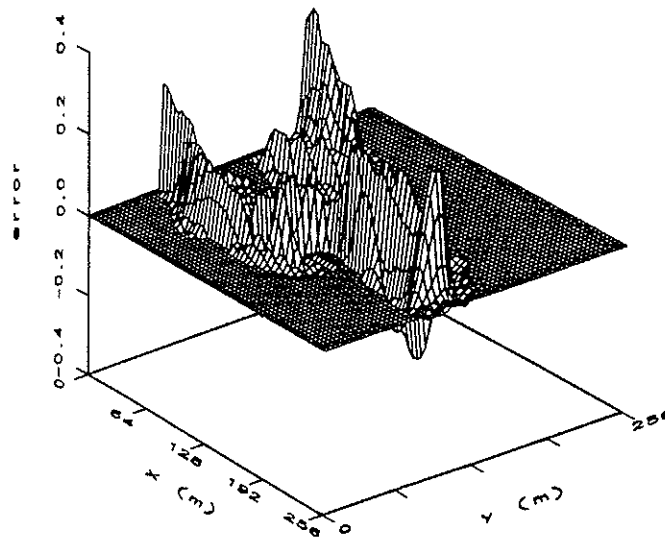


Figure 5. Coarse grid solution error in the second example plotted as difference between uniform coarse and uniform fine grid solutions at elapsed time of 1000 days.

Figure 6 shows the LAGR computational error relative to the uniform fine grid solution using a truncation error tolerance of 0.001, an efficiency of 80%, a buffer zone of one coarse grid block, and regridding every five coarse grid time steps. The errors are quite small. This performance is achieved at a computational cost of one quarter of the uniform fine grid cost.



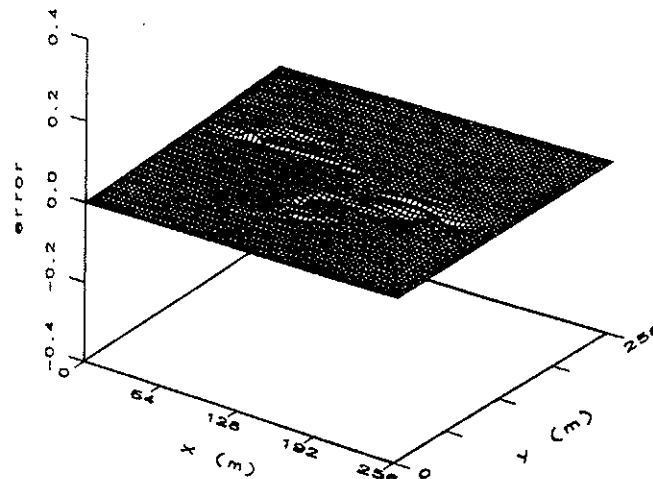


Figure 6. LAGR solution error for the second example plotted as difference between LAGR and uniform fine grid solutions at elapsed time of 1000 days.

Our final example involves competitive ion exchange between three species. The flow field is unidirectional through a homogeneous medium. The first species,  $M_1$ , is initially uniformly distributed throughout the domain and is at equilibrium, fully occupying all exchange sites. Solution and exchange site concentrations are both 0.5 mg/L. Species  $M_2$  and  $M_3$  are found initially only in a fixed concentration strip source with  $c_2 = c_3 = 1.0$  mg/L. The source is centered on the upstream boundary, and its length is equal to six-tenths of the width of the domain. As the two invader species move into the domain, they preferentially displace the sorbed phase of species 1. The equilibrium partitioning coefficients,  $K_{12}$  and  $K_{13}$ , are 2 and 4, respectively, so species 3 sorbs more readily than species 2, which in turn sorbs more readily than the resident species 1.

To demonstrate the performance of LAGR for this more chemically complex transport problem, solutions to the governing equations are computed on a uniform fine grid, a uniform coarse grid, and with LAGR. The spatial discretization on the coarse grid is 4 m and the time step is 5 days. The fine grid space and time steps are 1 m and 1.25 days. The preferential sorption leads to three different aqueous plumes. Figure 7 shows the dissolved concentration profiles after 1500 days, as simulated using LAGR.

A comparison of the uniform fine grid, uniform coarse grid, and the LAGR solutions is provided in Figure 8. The numerical error in the coarse grid solution is greatest in the region where competitive reactions occur between all three chemical species. The greater resolution on the uniform fine grid and LAGR subgrids reduces this numerical error. Once again, however, the LAGR solution is substantially more efficient, with a CPU time 28% that of the uniform fine grid.

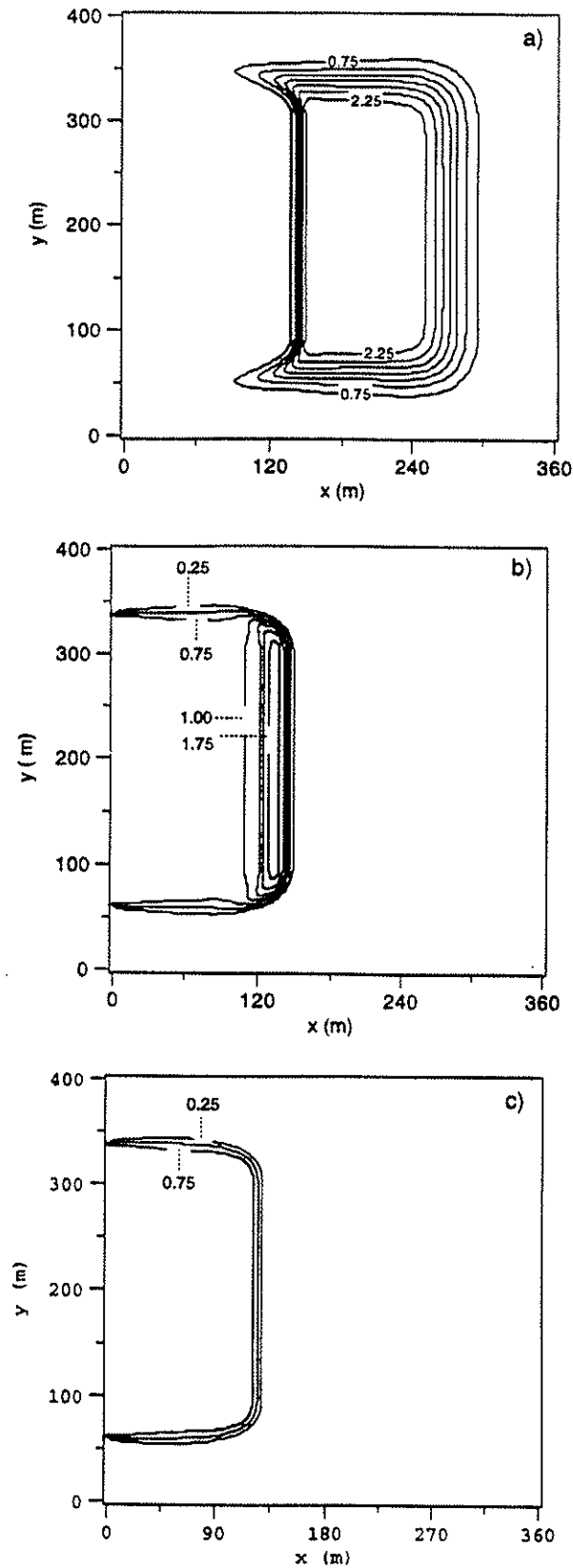


Figure 7. Solution concentration contours computed with LAGR in the third example problem at elapsed time of 1500 days for (a) species 1, (b) species 2, and (c) species 3. Concentrations in mg/L.

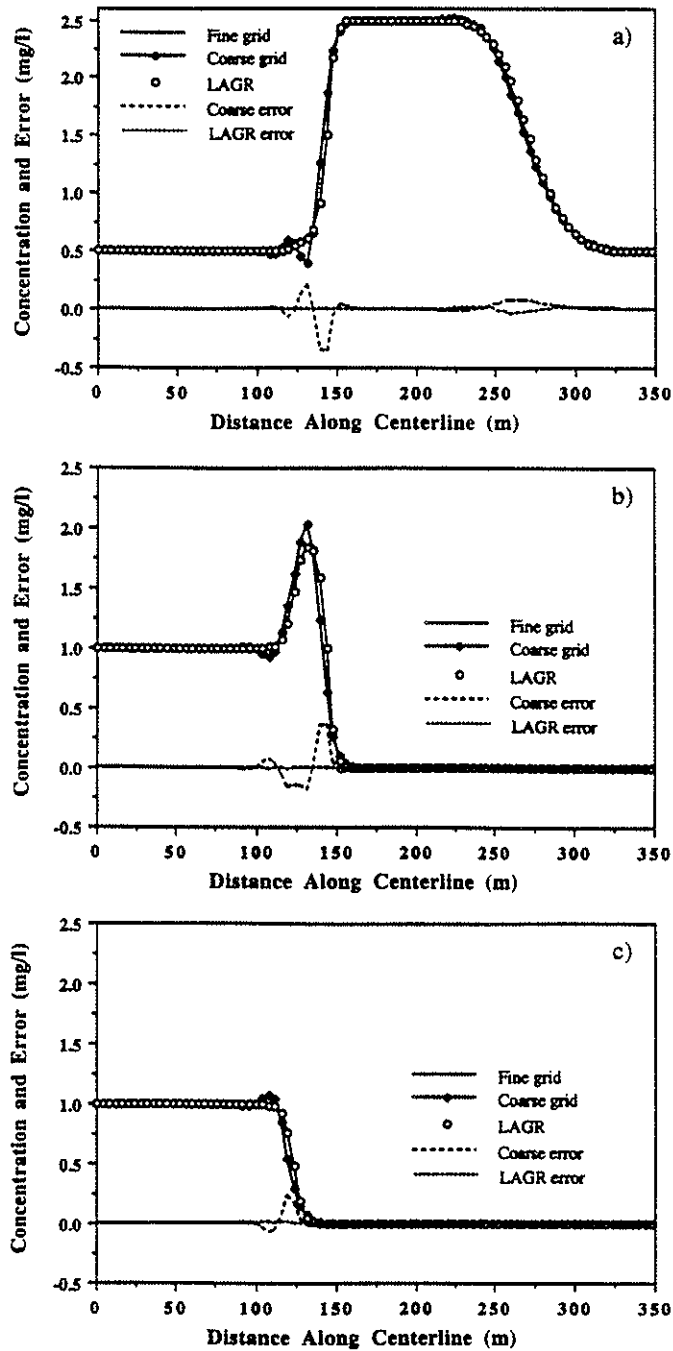


Figure 8. Comparison of uniform coarse grid, uniform fine grid, and LAGR solutions along the centerline ( $y = 200$  m) at elapsed time of 1500 days in the third example for (a) species 1, (b) species 2, and (c) species 3. Also shown is the concentration error for the uniform coarse grid and LAGR solutions relative to the fine grid solution.

## FINDINGS AND CONCLUSIONS

The local adaptive grid refinement method, LAGR, brings efficiency to accurate solutions of complex solute transport problems by supplying increased spatial and temporal resolution only as needed to otherwise coarse computational grids. Several novel features make the algorithm possible and widely applicable. First, estimates of the local truncation error at every node in the computational domain are calculated using the same solver which advances the solution. The process of computing the estimates is inexpensive relative to the simulation cost because only coarse grid solutions are required for the estimates. Then, subgrids with higher resolution than the original base grid are created and placed in regions of unacceptable numerical error. Solutions are computed on the subgrids and used to improve the base grid calculations. The computational burden associated with a LAGR simulation is split between the base grid calculations, the fine grid calculations, and the overhead associated with error estimation, subgrid generation, and grid communication.

Example problems demonstrate that LAGR achieves results similar to those obtained using a uniform fine grid at a fraction of the cost. For the example problems described earlier, solutions with accuracies comparable to those achieved with a uniform fine grid are obtained at between 20 and 30% of the computational cost.

Values of the LAGR design parameters (base grid discretization, truncation error tolerance, refinement ratio, minimum subgrid efficiency, buffer zone size, and regridding interval) determine the cost-accuracy trade-off. In general, there is no unique set of optimal parameter values. However, a few broad guidelines may be stated here, with more extensive analysis available in Wolfsberg (1993).

The coarse grid discretization defines the necessary solution resolution for interpreting the results of the simulation. The refinement ratio then defines the grid Peclet numbers for the subgrid computations. Knowledge of the accuracy of the particular solver as a function of grid Peclet number can assist in setting the refinement ratio. If multiple levels of refinement are allowed, then the refinement ratio assumes less importance in determining accuracy. The truncation error tolerance can be chosen via a conservative bound to limit the maximum solution error. Along with the truncation error tolerance, the buffer zone size and the regridding interval are most important in defining the solution cost-accuracy trade-off. Truncation error estimation and regridding are not required at every time step. The appropriate regridding interval is defined by the propagation speed of the concentration front(s) and the buffer zone size. If the size of the region undergoing refinement is known a priori, and the truncation error tolerance has been set, then a model can be formulated to predict approximately the appropriate buffer zone size and regridding interval to minimize computational costs. However, under usual circumstances, when the size of the refined region is not known a priori, there is no simple way to predict optimal values for these two parameters. A reasonable rule of thumb is to choose a buffer zone size of one or two coarse grid blocks and choose the regridding interval based on front propagation speed.

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**ADDITIONAL PROJECT PUBLICATIONS**

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