

# Subsurface transport modeling using adaptive finite elements

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## Abstract

A multi-dimensional finite element method (GWADAPT) which utilizes local mesh adaptation is used to calculate groundwater flow and subsurface transport of contaminant in saturated and unsaturated conditions. The model uses simple modifications to increase computational speed and reduce storage, allowing the model to run on PCs and workstations. GWADAPT can be accessed from the web and downloaded to a file. A parallel version of the model runs on an SGI Origin 2000 computer.

## 1 Introduction

Increasing emphasis is now being placed on the use of predictive computer models for regulatory and cleanup activities associated with groundwater flow and subsurface contaminant transport. Modeling such problems involves complicated physics, chemistry, and multi-phase flow phenomena, and typically requires the use of numerical techniques. A particularly attractive numerical scheme now being used to model subsurface transport is the finite element method (FEM).

Finite element codes have been used for many years to simulate transport of subsurface contaminant<sup>1,2</sup>. Early successes with the FEM in groundwater transport subsequently lead to increased application of the method.<sup>3-5</sup> Huyakorn and Wadsworth<sup>6</sup> developed a 3-D finite element model for fluid flow and solute transport in saturated or unsaturated porous media. Camp Dresser and McKee<sup>7</sup> used a 3-D finite element model and a random walk technique with Lagrangian particles to simulate tritium dispersion. Application of the FEM is rather commonplace today, and widely used for groundwater transport.<sup>8</sup> Two promising finite element codes now being used for assessing radioactive contaminant dispersion from former underground nuclear tests are FEFLOW<sup>9</sup>, a multi-dimensional code commercially available from Waterloo Geohydrologic and FEHM, a multi-dimensional code developed by Zobylovski et al<sup>10</sup> at Los Alamos National Laboratory.

The employment of adapting, unstructured meshes permits one to calculate difficult problems with a minimum of nodal points. Approaches in using FEM and mesh adaptation have been shown to be very successful for advection-dispersion problems.<sup>11,12</sup> The adaptive mesh algorithm lifts much of the burden of mesh generation from the user while increasing accuracy of the

results. Mesh adaptation is achieved using interpolation-based commands and averaging to refine/unrefine the mesh. Adapting meshes are especially effective for complex environmental problems, allowing one to obtain high accuracy with significantly reduced storage while minimizing computer time.<sup>13,14</sup>

GWADAPT is a multi-dimensional finite element model that incorporates local mesh refinement (h-adaptation) to calculate flow and species transport in saturated and unsaturated porous media. The code is written in C/C++/JAVA and runs on Pentium level PCs and workstations. The model employs Petrov-Galerkin weighting for the advection terms, mass lumping, reduced integration (when appropriate), and adaptive parameters based on velocities and/or concentration gradients. A parallel version of the code runs on the SGI Origin 2000 located at the University of Nevada, Las Vegas (UNLV). GWADAPT includes both pre- and post-processing capabilities, allowing the user to develop and modify mesh configurations as well as display results in real time. GWADAPT can be accessed directly from its UNLV web site at <http://www.nscee.edu/NCACM> and downloaded to a file.

## 2 Governing Equations

The governing equations for multi-dimensional, time dependent transport of contaminated groundwater flow in saturated porous media can be written in vector form as

$$R_d \frac{\partial C}{\partial t} + \mathbf{V} \cdot \nabla C = \nabla \cdot (\mathbf{D} \cdot \nabla C) + S \quad (1)$$

$$S_h \frac{\partial h}{\partial t} = \nabla \cdot (\mathbf{k} \cdot \nabla h) + Q \quad (2)$$

where  $C$  is the concentration,  $R_d$  is the retardation coefficient,  $\mathbf{V}$  is the vector velocity field,  $\mathbf{D}$  is the directionally dependent dispersion tensor,  $S$  (and  $Q$ ) represents source/sink terms (precipitation, radioactive decay, pumpage and recharge),  $h$  is the height of the water table above an impermeable base,  $S_h$  is specific yield, and  $\mathbf{k}$  is the tensor hydraulic conductivity.

The hydrodynamic dispersion tensor,  $\mathbf{D}$  ( $\equiv d_{ij}$ ) is defined as<sup>15</sup>

$$d_{ij} = \delta_{ij} \alpha_T |\mathbf{V}| + (\alpha_L - \alpha_T) \frac{\mathbf{V} \mathbf{V}^T}{|\mathbf{V}|} + \delta_{ij} \mu \quad (3)$$

where  $\alpha_L$  is the longitudinal dispersivity,  $\alpha_T$  is the transverse dispersivity,  $\delta_{ij}$  is the kronecker delta function, and  $\mu$  is the molecular diffusion coefficient.

Velocity components are determined from the relation

$$\mathbf{V} = -\mathbf{k} \cdot \nabla h / \theta \quad (4)$$

where  $\theta$  is effective porosity.<sup>16</sup>

For unsaturated porous media, the governing equations are

$$\frac{\partial C}{\partial t} + \mathbf{V} \cdot \nabla C = \nabla \cdot [\mathbf{D}(\psi) \cdot \nabla C] + S_\psi \quad (5)$$

$$C_\psi \frac{\partial \psi}{\partial t} = \nabla \cdot [\mathbf{k}(\psi) \cdot \nabla \psi] + Q_\psi \quad (6)$$

where  $\mathbf{D}(\psi)$  is the dispersion tensor based on the pressure head,  $\psi$  ( $\psi = h - z_o$ ),  $\mathbf{k}(\psi)$  is the tensor hydraulic conductivity,  $C_\psi$  is specific moisture capacity, and  $z_o$  is a reference depth.

Relations for  $\mathbf{D}(\psi)$  and  $\mathbf{k}(\psi)$  have been examined and studied for many years; the most popular expressions are discussed in Guymon.<sup>17</sup> One of the more popular relations stems from the work by van Genuchten (see Guymon<sup>17</sup>), and are used in a number of groundwater codes, i.e.,

$$\mathbf{k}(\psi) = k_s S_e^1 [1 - (1 - S_e^{1/m})^m]^2 \quad (7)$$

where  $k_s$  is saturated hydraulic conductivity,  $l$  is pore connectivity,  $m = 1 - 1/n$  where  $n$  is a best fit parameter, and  $S_e$  is reduced saturation based on porosity and water content. Since the equations for unsaturated flow are nonlinear, Picard iteration is used to achieve convergence for  $\mathbf{D}(\psi)$  and  $\mathbf{k}(\psi)$ .<sup>14</sup>

### 3 The finite element method

The finite element method is used as the basis for numerical implementation. Bilinear isoparametric quadrilateral and trilinear hexahedral elements are used to discretize a problem domain. Mesh generation in 2-D is achieved using GW\_MESH, which is a 2-D mesh generator package that accompanies GWADAPT; 3-D mesh generation is performed using TruGRID<sup>18</sup> and FEMGV<sup>19</sup>, two commercially available mesh generators.

The standard weak formulation of the Galerkin weighted residual technique is employed to cast the governing equations into their integral form. The Galerkin integral forms for Eqs. (1) and (2) are

$$\int_{\Omega} [W(R_d \frac{\partial C}{\partial t} + \mathbf{V} \cdot \nabla C - S) + \nabla W \cdot (\mathbf{D} \cdot \nabla C)] d\Omega - \int_{\Gamma} W \mathbf{n} \cdot (\mathbf{D} \cdot \nabla C) d\Gamma = 0 \quad (8)$$

$$\int_{\Omega} [W(S_h \frac{\partial h}{\partial t} - Q) + \nabla W \cdot (\mathbf{k} \cdot \nabla h)] d\Omega - \int_{\Gamma} W \mathbf{n} \cdot (\mathbf{k} \cdot \nabla h) d\Gamma = 0 \quad (9)$$

where  $W$  is the weighting function,  $\Omega$  is the computational domain with boundary  $\Gamma$ , and  $\mathbf{n}$  is the unit vector normal to  $\Gamma$ . The boundary integrals in Eqs. (8) and (9) arise from the application of Green's identity to the respective flux terms. The flux boundary conditions associated with both equations are readily satisfied through the natural boundary conditions of these expressions. Similar expressions are obtained for Eqs. (5) and (6).

The concentration and head are represented by the trial approximations

$$\hat{C}(\mathbf{x}, t) = \sum_{i=1}^n N_i(\mathbf{x}) C_i(t) \quad , \quad \hat{h}(\mathbf{x}, t) = \sum_{i=1}^n N_i(\mathbf{x}) h_i(t) \quad (10)$$

where  $\mathbf{x}$  denotes vector space and  $N_i(\mathbf{x})$  is the linear basis function associated with the  $i^{\text{th}}$  node of  $n$  total nodes in the mesh; in this instance,  $W \equiv N_i$  (except for advection).

The matrix equivalent forms of the resultant weak statements, Eqs. (8) and (9), can be expressed as

$$R_d[M]\{\dot{C}\} + [K_c]\{C\} + [A(\mathbf{V})]\{C\} = \{F_c\} \quad (11)$$

$$S_h[M]\{\dot{h}\} + [K_h]\{h\} = \{F_h\} \quad (12)$$

where the  $\dot{\phantom{x}}$  refers to time differentiation,  $M$ ,  $K$ , and  $A(\mathbf{V})$  are sparse matrix coefficients, and  $F_h$  and  $F_c$  are the right hand side vector loads. The matrix coefficients for Eqs. (11) and (12) are defined as

$$[M] = \int_{\Omega} N_i N_j d\Omega \quad , \quad [A(\mathbf{V})] = \int_{\Omega} W_i (\mathbf{V} \cdot \nabla N_j) d\Omega$$

$$[K_c] = \int_{\Omega} \nabla N_i \cdot (\mathbf{D} \cdot \nabla N_j) d\Omega \quad , \quad [K_h] = \int_{\Omega} \nabla N_i \cdot (\mathbf{k} \cdot \nabla N_j) d\Omega$$

$$\{F_c\} = \int_{\Omega} N_i S d\Omega + \int_{\Gamma} N_i \mathbf{n} \cdot (\mathbf{D} \cdot \nabla C) d\Gamma \quad , \quad \{F_h\} = \int_{\Omega} N_i Q d\Omega + \int_{\Gamma} N_i \mathbf{n} \cdot (\mathbf{k} \cdot \nabla h) d\Gamma$$

For steady state flow, the resulting Poisson equation for  $h$  is solved using Cholesky skyline decomposition. Simple modifications are used to replace the typical FEM global assembly operations with local formulations per time step.<sup>14</sup> When element distortion is minimal, reduced integration is used.

A Petrov-Galerkin scheme<sup>14</sup> is used to stabilize the species transport equation. In this approach, the advection term is weighted by the function

$$W_i = N_i + \frac{\alpha h_e}{2V} (\mathbf{V} \cdot \nabla N_i) \quad (13)$$

where  $h_e$  is calculated using the mesh length vectors and  $\alpha = \coth \beta/2 - 2/\beta$  with  $\beta = |V|h_e/2D_e$ . The coefficient  $D_e$  is an effective diffusion in the direction of the local velocity vector and is calculated from the relation

$$D_e = \frac{\mathbf{V}^T \cdot \mathbf{D} \cdot \mathbf{V}}{|\mathbf{V}|^2} \quad (14)$$

This weighting has the effect of introducing a form of anisotropic balancing diffusion into the numerical scheme that acts along the local streamline.

The mass matrix  $[M]$  is diagonalized by employing a lumped mass

approximation

$$[M^1] = \int_{\Omega} N_i \left( \sum_{j=1}^n N_j \right) d\Omega \quad (15)$$

where all off-diagonal terms of the lumped mass matrix are zero. An explicit second-order Runge-Kutta method is used to advance the discretized equations in time. The concentration,  $\{C\}$ , is advanced in time according to the following two-step algorithm:

$$\begin{aligned} \{C\}^{n+1/2} &= \{C\}^n + \frac{\Delta t [M^1]^{-1}}{2R_d} [\{F_c\} - ([K_c]\{C\} - [A(\mathbf{V})]\{C\})^n] \\ \{C\}^{n+1} &= \{C\}^n + \frac{\Delta t [M^1]^{-1}}{2R_d} [\{F_c\} - ([K_c]\{C\} - [A(\mathbf{V})]\{C\})^{n+1/2}] \end{aligned} \quad (16)$$

where superscript  $n$  denotes a quantity evaluated at time  $n\Delta t$ , with  $\Delta t$  being the magnitude of the time step. Courant limits associated with a forward Euler scheme are calculated over each element, and the time step adjusted to the minimum value within the computational domain.

#### 4 Mesh Adaptation

In h-adaptation, the computational mesh refines and unrefines by adding and subtracting elements within the computational domain as the solution evolves in time. The number of elements (and node points) are increased in regions of high gradients, and reduced where the flow is smooth. However, the overall number of nodes and elements increases - keeping track of new nodes and element connectivity can become cumbersome.

A coarse mesh is initially generated which will allow enough transport details to appear and yet yield convergence. A preliminary solution (not converged) is computed on the crude mesh, and refinement indicators calculated based on the first difference of concentration within each element. Elements that need to be refined or unrefined are identified; refinement proceeds from the coarsest level to the finest level. The adaptive refinement threshold values are generally determined empirically; these values can be varied to cause more or less elements to be refined or unrefined, depending upon desired accuracy and computer time.

After all the mesh changes have been made, the grid geometry is recalculated, the solution is interpolated onto the new grid, and the calculation procedure begun again. The calculation procedure continues until the concentration converges to a criterion of  $10^{-4}$ . In transient problems, the mesh is adapted to capture high gradient features as they evolve in time. A more detailed description of the adaptation process is discussed in Pepper and

Stephenson.<sup>14</sup> An example of 3-D mesh adaptation is shown in Fig. 1.

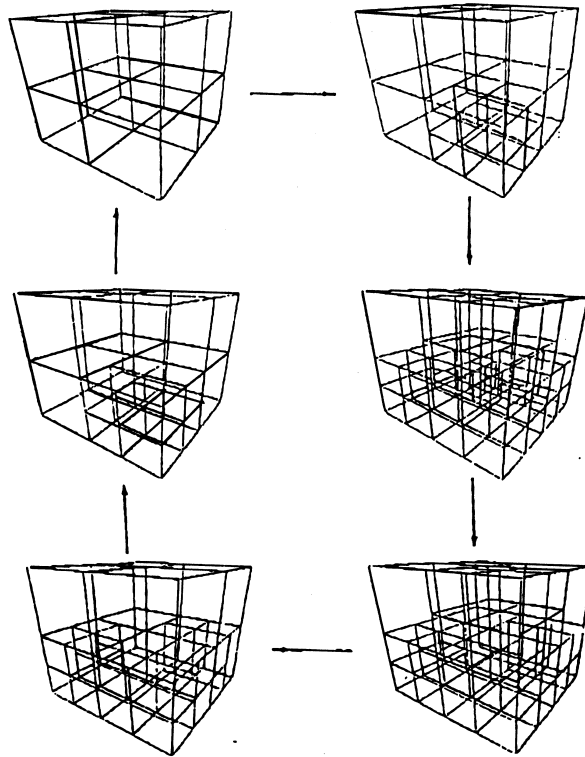


Figure 1. 3-D Mesh Adaptation

## 5 Model Results

Considering a vertical flow domain that describes the contaminant influence on a discharging aquifer from a leaking contaminant deposit. The cross-sectional domain has a length of 1000 m and a height of 40 m, as shown in Fig. 2. The aquifer is discharged from left to right. The deposit contacts the aquifer on the top over a length of 50 m, where contaminant matter is released. The isotropic hydraulic conductivity is  $10^{-4}$  m/s, the porosity is 0.3, the molecular diffusion is  $10^{-9}$  m<sup>2</sup>/s, the longitudinal dispersivity is 2 m, and the transverse dispersivity is 0.1 m. The inflow boundary has a constant influx of 0.1 m/d and the outflow boundary has a constant hydraulic head of 40 m. The flow boundary condition of the leaking deposit has a constant influx of 0.0125 m/d. Isopleth concentration contours using three levels of adaptation are shown in Fig. 3. Unsaturated conditions are that the volume moisture content is 0.3 and the volume saturation is 0.5. Isopleth concentration contours for unsaturated conditions are shown in Fig. 4. Three-dimensional results using FEFLOW for saturated groundwater are shown in Figs. 5 and 6 and show good agreements between Figs. 3 and 5, and Figs. 4 and 6, as shown in Table 1.

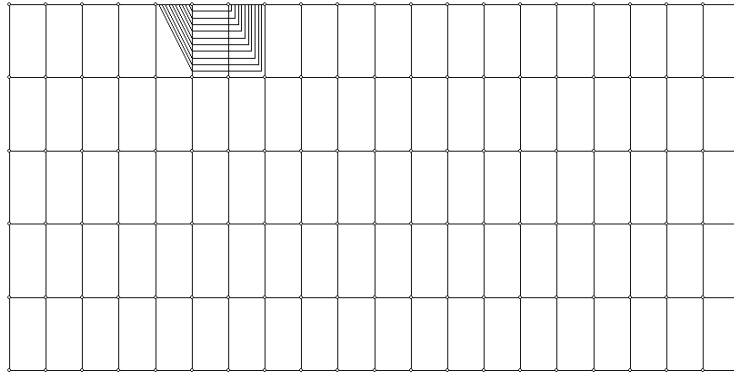


Figure 2. Cross-section domain of a leaking contaminant deposit.

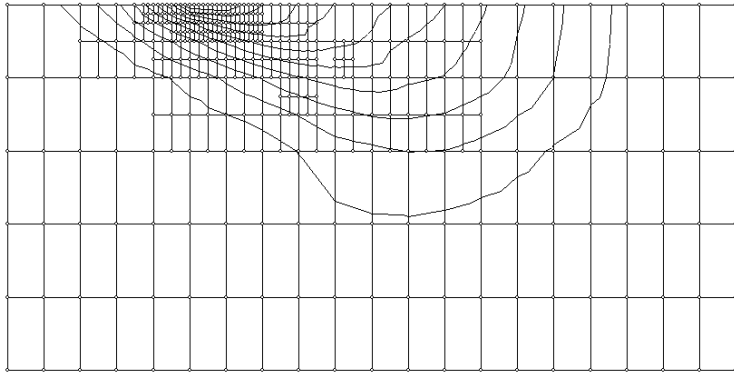


Figure 3. Concentration contours from a leaked deposit with a three-level mesh h-adaptation in the saturated groundwater at 30 days.

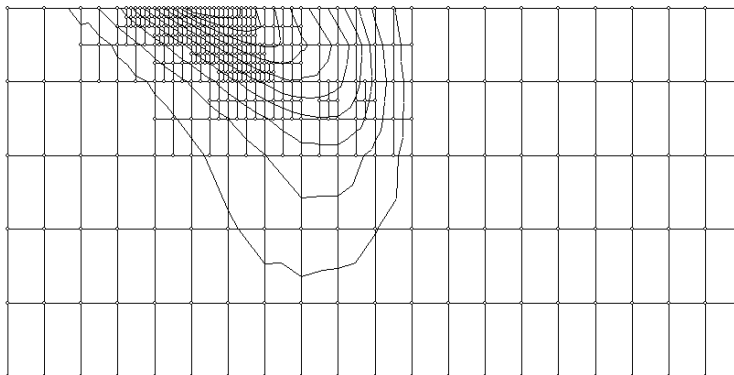


Figure 4. Concentration contours from a leaked deposit with a three-level mesh h-adaptation in the unsaturated groundwater at 5500 days.

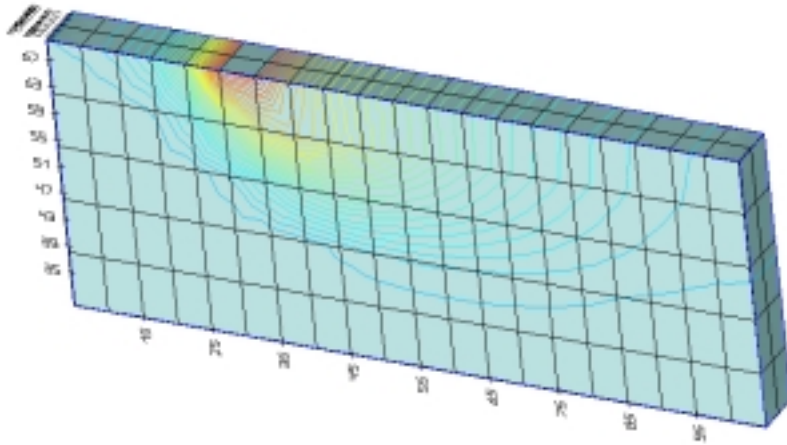


Figure 5. Concentration contours from a leaked deposit using FEFLOW in the saturated groundwater at 30 days.

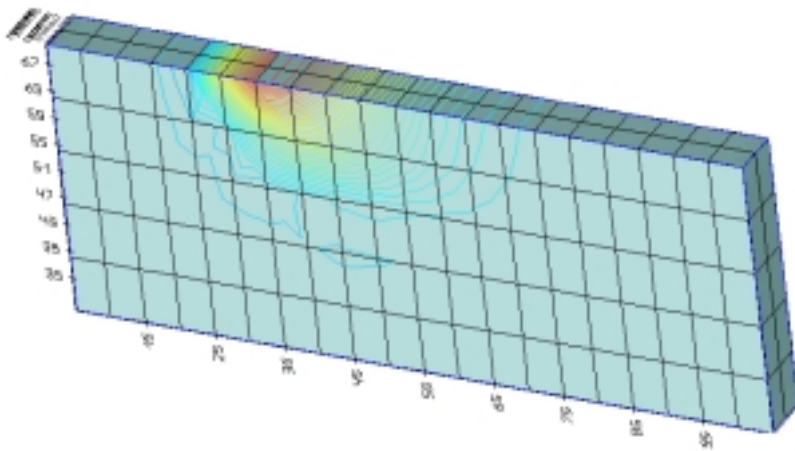


Figure 6. Concentration contours from a leaked deposit using FEFLOW in the unsaturated groundwater at 5500 days.

Table 1. Comparisons between GWAdapt and FEFLOW for saturated and unsaturated flow

	GWAdapt		FEFLOW	
	(250m, 8m)		(250m, 8m)	
	saturated	unsaturated	saturated	unsaturated
Concentration (mg/l)	0.061743	0.13048	0.0636	0.1174
Velocity (x-zdirection)(m/d)	0.094938	0.004016	0.0978	0.0043



## 6 Parallel Processing – SGI Origin 2000

Large-scale, 3-D flowfield and transport resolution typically require a large number of nodes to discretize a problem domain. The resulting computational effort can quickly become inhibiting when running on a single processor machine. A simulation modeling the transport of contaminants for long periods of time can require large amounts of memory and CPU time. Earlier work with a similar algorithm by Pepper et al<sup>20</sup> using a MasPar 1216 SIMD computer with 16,384 processors also showed dramatic improvement in computing speed using FORTRAN 90 conversion.

The scalar version of GWADAPT was modified and rewritten to run on the SGI Origin 2000 parallel computer. Much of this effort required changing the Cholesky solver for the implicit solution of steady-state head values to be more efficient when running on multiple processors. After some trial and error, speed-ups on the order of 3-4 were obtained after partitioning the solution over ten processors. Several implicit solvers also exist that have been optimized for the SGI Origin 2000; two of the solvers worth looking into are the sparse Cholesky solver developed by Ng<sup>21</sup> at Oak Ridge National Laboratory and a direct solver developed at NASA Langley Research Center (see Storaasli<sup>22</sup>).

## 7 Conclusion

The incorporation of local mesh adaptation into finite element methods produce a very powerful and accurate numerical scheme for solving transport problems. Although the bookkeeping associated with keeping track of the refined and unrefined elements can be troublesome, the end result is well worth the effort. GWADAPT is a finite element code that uses h-adaptation to calculate groundwater flow and species transport in saturated or unsaturated porous media. The model is written in C/C++/JAVA and incorporates pre- and postprocessors for mesh generation and visualization of results in real time. GWADAPT can be accessed from the web, allowing anyone interested in using the code to quickly use it to model subsurface transport. GWADAPT has been shown to be very accurate, and is quite easy to use even though it is a very robust program.

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