Application of Discrete Sensitivity Analysis
to Water Resource Applications

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May 3, 2000

Abstract

Discrete sensitivity analysis is a method that efficiently estimates the derivatives of a numerically approximated objective function with respect to a set of parameters. This method can be coupled with an optimization algorithm to locate the optimal set of parameters for the objective function. Many problems within water resource applications are studied via numerical simulations and can be re-formulated into function optimization problems. Two examples, which are presented in this paper, are the design of open-channels using a two-dimensional Petrov-Galerkin finite element code and the identification of parameters for a time-dependent, two-dimensional groundwater code. Once these problems are formulated into optimization problems, the steady and unsteady adjoint variable formulation of discrete sensitivity analysis are used to estimate the gradient, and the BFGS optimization algorithm is used to update the parameters.

1 Introduction

A wide variety of engineering problems within water resource applications can be formulated as a function minimization problem, subject to constraints. For instance, the design of storm-water management systems requires that each open-channel in the system provide for a large discharge of water without causing floods. Each transition region could be optimized by changing the shape of the open channel to minimize the average depth of water in channel. Another example is in parameter estimation within groundwater aquifers. In this case, the optimal set of parameter could be estimated by minimizing the difference between the computed pressures within the aquifer and the observed pressures, as water is being pumped out of the aquifer or into the aquifer. By working alongside engineers in the field, the goals of a particular engineering project and the restrictions can be ascertained, and appropriate objective and constraint functions, as well design parameters, can be determined.

Once the optimization problem has been defined, numerical methods can be employed to evaluate a particular design (i.e., evaluate the objective function), to determine the sensitivities of the design with regards to the various parameters (i.e., estimate the gradient of the objective function) and to modify the design based on the sensitivities (i.e., update the design parameters). With the development of greater computing power and high-fidelity computational fluid dynamics, better numerical methods for evaluating the flow through a particular design are continuing to be developed. Using the appropriate numerical tool, the merits of a particular design can be evaluated.

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To estimate the sensitivities of the design with respect to the parameters, the researcher can use a variety of numerical methods, including finite differences, automatic differentiation, the complex Taylor's series expansion method and discrete or continuous sensitivity analysis. For high-fidelity, implicit flow solvers, discrete sensitivity analysis provides accurate derivative information efficiently. Both the steady-state and unsteady adjoint variable formulations of discrete sensitivity analysis will be presented herein.

Once the design has been evaluated and the sensitivities have been determined, the design parameters should be updated. The method of steepest descent moves the parameters in the gradient direction, which is easy to implement, but often performs poorly. Quasi-Newton methods, such as the BFGS secant update method, use only gradient information to build an approximation to the Hessian matrix, which provides for much better convergence rates. For direct methods, the Gauss-Newton method also provides superlinear convergence rates and may be more successful that Quasi-Newton methods.

In the next section, the author will give a brief background to the use of sensitivity analysis within gradient-based numerical design optimization. In the remainder of this paper, the author will present the steady-state formulations of discrete sensitivity analysis and apply these techniques to a two-dimensional, finite element, shallow water solver for flow through an open-channel. Then the author will describe the unsteady, adjoint formulation and apply the method to groundwater parameter estimation.

2 Background

Both discrete and continuous sensitivity analysis have been used to convert CFD codes into gradient estimation codes in a variety of fields, including aerospace simulations and water resources. Within the aerospace field, Jameson and Reuther [1,2] were some of the early advocates of continuous sensitivity analysis, and Shubin and Frank [4], Taylor and Hou [5] and Baysal and Eleshaky [6] were some of the first researchers with discrete sensitivity analysis. Soemarwoto [3] gives an excellent analysis of continuous sensitivity analysis which will not be repeated here.

With regard to open-channel flow and river analysis problems, Piasecki and Katopodes [7] used continuous sensitivity analysis to determine the sensitivities of contaminant concentrations with respect to times and rates of contaminant releases from industrial facilities. Khatibi, etal [8], used continuous sensitivity analysis to estimate friction coefficients for the one-dimensional St. Venant equations, and Atanov, etal [9], used the continuous approach to determine the temporal controls for the upstream gate on a channel. Burg, etal [10], have used discrete sensitivity analysis for a two-dimensional code to design open-channels that produce minimal downstream disturbances.

For groundwater modeling, Townley and Wilson [11] developed the time-dependent discrete sensitivity equations, which will be presented again in this paper, for use within groundwater analysis. This work was published in 1985 and represents a significant contribution that may have been overlooked by other researchers. Due to the difficulties inherent in groundwater modeling, including the simulation of the physical effects, such as leaky aquifers and aquifer recharge effects, and the determination of severely localized groundwater parameters, application of continuous and discrete sensitivity analysis to groundwater modeling is an underdeveloped field of research.

3 Steady Discrete Sensitivity Analysis

Using an implicit solution algorithm, such as a finite element or finite volume method, marching in time towards the steady-state solution, the flow variables at time level n are updated based on the solution of the following equation

$$\left[\frac{\partial R}{\partial Q}\right] \Delta Q^{n,m} = -R(Q^{n,m}, \chi(\vec{\beta}), \vec{\beta}, t^n) \tag{1}$$

where $R(Q, \chi(\vec{\beta}), \vec{\beta}, t)$ is the residual vector of the time-dependent equations, Q is a vector of flow variables, χ is a vector of nodal locations within the computational domain, $\vec{\beta}$ is a vector of design parameters that can control the shape of the design or the flow parameters. The matrix $\left[\frac{\partial R}{\partial Q}\right]$ is either the exact Jacobian matrix of the residual with respect to the flow variables, or it is an approximation to this matrix. After solving this equation, the flow variables are updated via $Q^{n,m+1} = Q^{n,m} + \Delta Q^{n,m}$, until $|\Delta Q^{n,m}| <$ tolerance, at which point $Q^{n+1} = Q^{n,m+1}$.

Once they are determined, the steady-state flow variables Q are dependent on the grid χ and the design parameters $\vec{\beta}$, and the residual can be expressed as

$$R(Q(\chi(\vec{\beta}), \vec{\beta}), \chi(\vec{\beta}), \vec{\beta}) = 0 \tag{2}$$

Suppressing the dependence on χ, since the grid can be determined from the design parameters, the residual can be expressed as

$$R(Q(\vec{\beta}), \chi(\vec{\beta}), \vec{\beta}) = 0 \tag{3}$$

The objective function $F(Q(\vec{\beta}), \chi, \vec{\beta})$ is typically an analytic function of the flow variables Q, the grid χ and the design parameters $\vec{\beta}$. The total variation of F with respect to the design parameter β_k is

$$\frac{dF}{d\beta_k} = \frac{\partial F}{\partial Q}\frac{\partial Q}{\partial \beta_k} + \frac{\partial F}{\partial \chi}\frac{\partial \chi}{\partial \beta_k} + \frac{\partial F}{\partial \beta_k} \tag{4}$$

The vectors $\frac{\partial F}{\partial Q}$, $\frac{\partial F}{\partial \chi}$ and $\frac{\partial F}{\partial \beta_k}$ can be readily determined from the analytic expression for F. The vector $\frac{\partial \chi}{\partial \beta_k}$ can be obtained by perturbing the design parameters, regenerating the grids and calculating the change in the nodal locations. The vector $\frac{\partial Q}{\partial \beta_k}$ can also be obtained by perturbing the design parameters and calculating the flow through the new design, but as this method would require several additional steady-state simulations, it could be excessively expensive.

The total variation of the residual with respect to any variable is zero, because it is an implicitly defined function. Thus,

$$\frac{dR}{d\beta_k} = \left[\frac{\partial R}{\partial Q}\right]\frac{\partial Q}{\partial \beta_k} + \left[\frac{\partial R}{\partial \chi}\right]\frac{\partial \chi}{\partial \beta_k} + \frac{\partial R}{\partial \beta_k} = 0 \tag{5}$$

This equation can be rewritten as

$$\left[\frac{\partial R}{\partial Q}\right]\frac{\partial Q}{\partial \beta_k} + \left.\frac{dR}{d\beta_k}\right|_{Q \text{ fixed}} = 0 \tag{6}$$

The matrix $\left[\frac{\partial R}{\partial Q}\right]$ is already available within an implicit code. The vector $\left.\frac{dR}{d\beta_k}\right|_{Q \text{ fixed}}$ can be obtained with relative efficiency by finite differences. Thus, we have an equation for the troublesome vector $\frac{\partial Q}{\partial \beta_k}$.

The adjoint variable formulation multiplies equation (6) by an adjoint vector λ and adds the result to equation (4), which yields

$$\frac{dF}{d\beta_k} = \left(\frac{\partial F}{\partial Q} + \lambda^T\left[\frac{\partial R}{\partial Q}\right]\right)\frac{\partial Q}{\partial \beta_k} + \frac{\partial F}{\partial \chi}\frac{\partial \chi}{\partial \beta_k} + \frac{\partial F}{\partial \beta_k} + \left.\frac{dR}{d\beta_k}\right|_{Q \text{ fixed}} \tag{7}$$

By choosing λ such that

$$\frac{\partial F}{\partial Q} + \lambda^T\left[\frac{\partial R}{\partial Q}\right] = 0 \tag{8}$$

the need to calculate the vector $\frac{\partial Q}{\partial \beta_k}$ is removed. Thus, the adjoint variable equation is

$$\left[\frac{\partial R}{\partial Q}\right]^T \lambda = -\frac{\partial F}{\partial Q} \tag{9}$$

This equation is not dependent on the design parameter β_k, but does depend on the objective function F. Thus, the adjoint variable equation must be solved once for each objective function, without regard to the number of design parameters.

The direct approach solves equation (6) directly for $\frac{\partial Q}{\partial \beta_k}$, or

$$\left[\frac{\partial R}{\partial Q}\right]\frac{\partial Q}{\partial \beta_k} = -\left.\frac{dR}{d\beta_k}\right|_{Q \text{ fixed}} \tag{10}$$

This equation depends on the design parameter and must be solved once for each design parameter, regardless of the number of objective functions. Thus, when the number of design parameters exceeds the number of objective and constraint functions, then the adjoint variable formulation is more computational efficient.

4 Steady State Example

For an example using a steady-state code to evaluate a design and to estimate the sensitivities of the design, a two-dimensional, Petrov-Galerkin, finite element solver of the shallow water equations for flow through open-channels is used. The shallow water equations are reliable when the vertical velocities in the flow are negligible. For slopes that are geometrically mild, albeit hydraulically steep, such as in concrete-lined open channels, this restriction is not violated as long as there is not a hydraulic jump in the flow. For more details about the flow solver HIVEL2D, the interested reader is referred to the work of Berger and Stockstill [12,13], and for information about the shallow water equations, the reader is referred to the work of Chaudhry [14].

The design problem is to identify the optimal slope of the bed across the channel before, through and after a circular channel, so as to maintain a constant surface elevation. The channel discharge rate is $43.794 m^3/sec$, the slope in the direction of flow is 0.012, and the Froude number is 2.387. The channel makes a 90^o turn to the right. The objective function is

$$F(\vec{\beta}) = \sum_{i=1}^{NROWS} \sum_{j=Column1}^{Column2} \left(h_{ave} - h_{i,j})^2 \right) \tag{11}$$

where h_{ave} is the average depth over the domain of the objective function and $h_{i,j}$ is the depth at each node within the domain. There were 50 design parameters that were the control points for a B-Spline curve that determined the slope across the channel.

The adjoint variable formulation of discrete sensitivity analysis was used to estimate the sensitivities. The resulting derivatives for several of the design variables are compared with the numerically exact derivatives as generated via the complex Taylor's series expansion method [15,16] and are presented in Table 1. From these derivatives, one can assume that the derivatives are accurate to between 6 and 8 significant digits. By obtaining such high level of agreement, the researcher can be confident that the majority of the implementation errors have been eliminated and that the derivatives will be similarly accurate throughout the optimization process.

Design Variable	Discrete Sensitivity Analysis	Numerically Exact Derivative
1	19.964851067446	19.964852378709
2	25.108134826382	25.108134714268
3	19.358701999683	19.358691597705
10	-12.677576340546	-12.677577631453
18	-32.637833170140	-32.637829687631
25	16.151752162457	16.151750639481
33	-18.134686276300	-18.134684699045
40	-5.0942054245774	-5.0942074466819
47	-5.3103160489289	-5.3103194084512
50	0.37009624729716	0.37009561184092

Table 1. Comparison of Sensitivities for Circular Channel Bend.

The computational cost of estimating the sensitivities via the adjoint variable formulation for the initial iteration, which includes the steady-state simulation, is 5240.72 seconds, whereas the cost for generating the numerically exact derivatives was 110,138.625 seconds. Thus, the adjoint variable formulation was significantly more efficient, requiring only 4.75% of the computational cost of the numerically exact method.

The BFGS Optimization algorithm [17] was used to update the design parameters. After 9 iterations, the function value has decreased by 99.84%. The convergence history is shown in Figure 1. The flow field for the initial design, where the slope across the channel is zero, and for the final design are given in Figures 2 and 3.

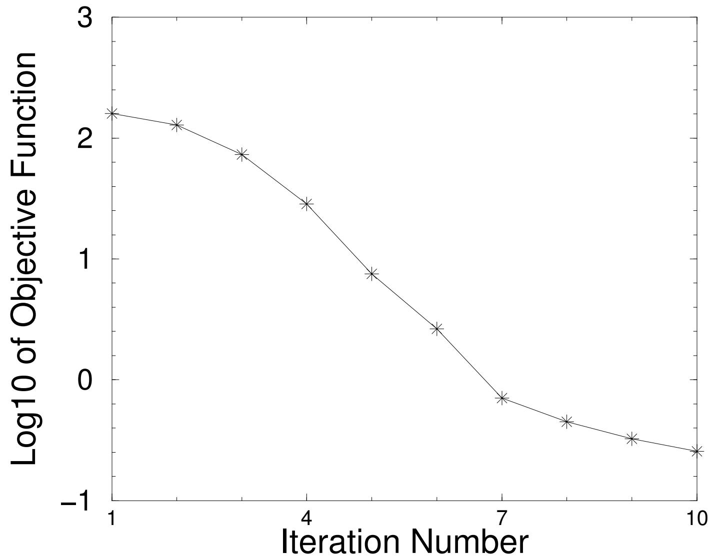

Figure 1. Convergence History.

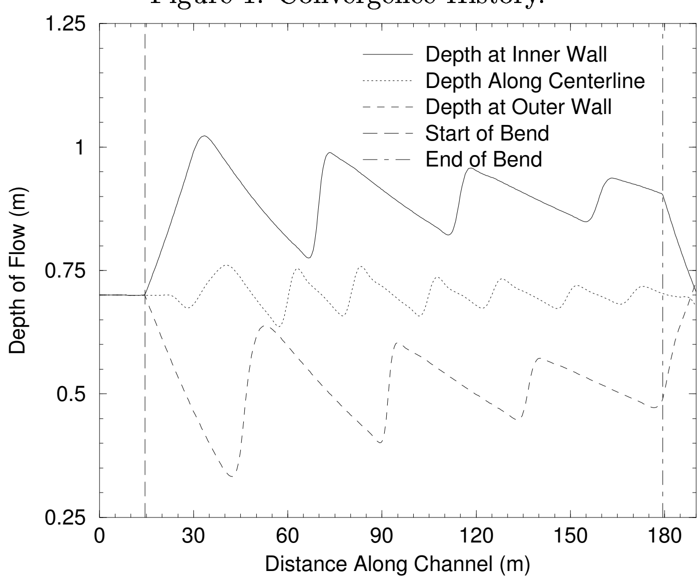

Figure 2. Flow Field for Initial Design.

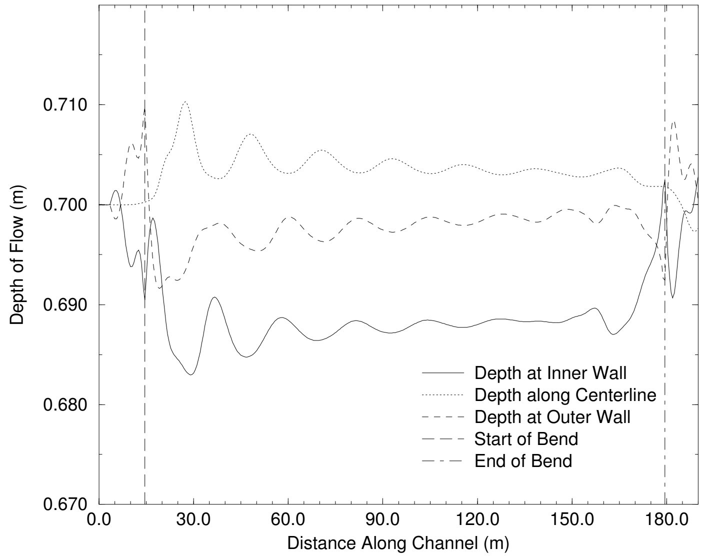

Figure 3. Flow Field for Final Design.

In Figure 2, the flow field for initial design have several waves that bounce back and forth across the bend and continue to exert a significant influence far downstream of the bend. Once the channel bend begins, the flow on the inner wall drops down to half the original water level, while the flow on the outer wall increases by 50%, which could result in the water overtopping the walls and cause flooding. For the converged design, the water levels are not perfectly constant, but rather than fluctuating at almost 50% of the initial depths, it stays within a band of about 4%, greatly reducing the dangers of flooding.

5 Unsteady Discrete Sensitivity Analysis

For unsteady problems, the objective function is evaluated at several time levels, so it can be expressed as

$$F(\vec{\beta}) = \sum_{n=1}^{N} f_n(Q^n(\vec{\beta}), \chi(\vec{\beta}), \vec{\beta}) \tag{12}$$

where the time levels are indicated by the index n. At each time level, the temporal residual is driven to zero, so that the flow variables at time level n are determined by solving

$$R^n(Q^n, Q^{n-1}, \chi, \vec{\beta}) = 0 \tag{13}$$

where Q^n is the vector of unknowns and Q^{n-1} is the vector of flow variables at the previous time level, which is already known. If the flow variables at other time levels are necessary, then the equation can be accommodated for them.

The total variation of the objective function with respect to a design parameter is

$$\frac{dF}{d\beta_k} = \sum_{n=1}^{N} \left(\frac{\partial f_n}{\partial Q^n} \frac{\partial Q^n}{\partial \beta_k} + \frac{\partial f_n}{\partial \chi} \frac{\partial \chi}{\partial \beta_k} + \frac{\partial f_n}{\partial \beta_k} \right) \tag{14}$$

At time level n, the derivative of the residual vector is

$$0 = \frac{dR}{d\beta_k} = \frac{\partial R^n}{\partial Q^n} \frac{\partial Q^n}{\partial \beta_k} + \frac{\partial R^n}{\partial Q^{n-1}} \frac{\partial Q^{n-1}}{\partial \beta_k} + \frac{\partial R^n}{\partial \chi} \frac{\partial \chi}{\partial \beta_k} + \frac{\partial R^n}{\partial \beta_k} \tag{15}$$

For each time level, the derivative of the residual vector is multiplied by the adjoint vector λ_n and added to the derivative of the function to get

$$\begin{aligned} \frac{dF}{d\beta_k} &= \sum_{n=1}^{N} \left(\frac{\partial f_n}{\partial Q^n} \frac{\partial Q^n}{\partial \beta_k} + \frac{\partial f_n}{\partial \chi} \frac{\partial \chi}{\partial \beta_k} + \frac{\partial f_n}{\partial \beta_k} \right) \\ &+ \sum_{n=1}^{N} \left({\lambda_n}^T \frac{\partial R^n}{\partial Q^n} \frac{\partial Q^n}{\partial \beta_k} + {\lambda_n}^T \frac{\partial R^n}{\partial Q^{n-1}} \frac{\partial Q^{n-1}}{\partial \beta_k} + {\lambda_n}^T \frac{\partial R^n}{\partial \chi} \frac{\partial \chi}{\partial \beta_k} + {\lambda_n}^T \frac{\partial R^n}{\partial \beta_k} \right) \end{aligned} \tag{16}$$

By regrouping the terms $\frac{\partial Q^n}{\partial \beta_k}$, the equation can be rewritten as

$$\begin{aligned} \frac{dF}{d\beta_k} &= {\lambda_1}^T \frac{\partial R^1}{\partial Q^o} \frac{\partial Q^o}{\partial \beta_k} + \sum_{n=1}^{N-1} \left(\frac{\partial f_n}{\partial Q^n} + {\lambda_n}^T \frac{\partial R^n}{\partial Q^n} + {\lambda_{n+1}}^T \frac{\partial R^{n+1}}{\partial Q^{n+1}} \right) \frac{\partial Q^n}{\partial \beta_k} \\ &+ \left(\frac{\partial f_N}{\partial Q^N} + {\lambda_N}^T \frac{\partial R^N}{\partial Q^N} \right) \frac{\partial Q^N}{\partial \beta_k} + \sum_{n=1}^{N} \left(\frac{\partial f_n}{\partial \chi} \frac{\partial \chi}{\partial \beta_k} + \frac{\partial f_n}{\partial \beta_k} + {\lambda_n}^T \frac{\partial R^n}{\partial \beta_k} \right) \end{aligned} \tag{17}$$

Thus, by solving the following equations, the adjoint vectors λ_n can be determined, and the need to estimate the vectors $\frac{\partial Q^n}{\partial \beta_k}$ is removed.

$$\frac{\partial f_N}{\partial Q^N} + {\lambda_N}^T \frac{\partial R^N}{\partial Q^N} = 0 \tag{18}$$

and

$$\frac{\partial f_n}{\partial Q^n} + {\lambda_n}^T \frac{\partial R^n}{\partial Q^n} + {\lambda_{n+1}}^T \frac{\partial R^{n+1}}{\partial Q^{n+1}} = 0 \tag{19}$$

Rewriting them, we get

$$\frac{\partial R^N}{\partial Q^N}^T \lambda_N = -\frac{\partial f_N}{\partial Q^N}^T \tag{20}$$

and

$$\frac{\partial R^n}{\partial Q^n}^T \lambda_n = -\frac{\partial f_n}{\partial Q^n}^T - \frac{\partial R^{n+1}}{\partial Q^{n+1}}^T \lambda_{n+1} \tag{21}$$

From these equations, it is clear that the adjoint vectors must be determined by going backwards in time. The first adjoint vector to be determined is at time level N and each further adjoint vector is determined by using the known adjoint vector at the next time level. For the initial time level, the dependence of the flow variables Q^o on the design parameter β_k should be explicitly known and the term $\lambda_1 \frac{\partial R^1}{\partial Q^o} \frac{\partial Q^o}{\partial \beta_k}$ can be determined once λ_1 is calculated. In many cases, $\frac{\partial Q^o}{\partial \beta_k}$ will be zero.

Once the adjoint vectors are determined, the sensitivities can be determined by calculating $\frac{\partial R^n}{\partial \beta_k}$ for each time level and each design variable.

Because a finite element formulation is used to integrate the governing equations, second order accuracy can be achieved for both the residual vector R and the Jacobian matrix $\frac{\partial R}{\partial Q}$, so that these two components of the adjoint equations are consisted with each other. If approximations are used within the Jacobian matrix, then additional errors will be introduced into the sensitivities generated by the adjoint variable formulation. By using a more accurate Jacobian, as generated via finite differences or the complex Taylor's series expansion method [18], these errors can be reduced significantly.

6 Unsteady Example

To demonstrate the unsteady adjoint variable formulation of discrete sensitivity, this method was applied to a time-dependent, unstructured code that solves the two-dimensional porous media equation for confined, heterogeneous aquifers and allows multiple, variable pumping rate wells. The porous media equation can be expressed as

$$S\frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left(T\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(T\frac{\partial h}{\partial y}\right) + \text{Pumping Terms} \tag{22}$$

where h is the hydraulic head within the aquifer, S is the storage coefficient and T is the transmissivity, both of which can vary in space. The Galerkin finite element method is used to integrate these equations over an unstructured grid that has a refined grid near the wells and a coarse grid far from the wells. The code was verified against analytic solutions of the steady-state equations and against the Theis solution for unsteady isotropic flow.

For the hydraulic engineer who is attempting to understand the structure of the aquifer, some of the key pieces of information to this structure are the pumping rates and the drawdown curves at each pumping well and the drawdown curves at each observation well. An optimization problem can be developed for solving for the storage coefficient and transmissivity throughout the computational domain by minimizing the objective function

$$F(T,S) = \sum_{i=1}^{N_t}\left(\sum_{j=1}^{N_w}\left(h_{i,j}^{\text{measured}} - h_{i,j}(S,T)\right)^2\right) \tag{23}$$

where i is the index for the time level, j is the index for the wells, $h_{i,j}^{\text{measured}}$ are the measured or target values, and $h_{i,j}(S,T)$ are the computed values for a specified set of storage coefficients and transmissivities.

To reduce the size of the search space, a parameter grid with substantially fewer nodes was used to define the values of S and T throughout the domain and the nodal values for the computational domain were determined via linear interpolation from these values. The target depths were determined by specifying a set of storage coefficients and transmissivities and then calculating and storing the depths generated by these values. For the target depths, the storage coefficient varied from 10^{-5} and 10^{-2}, while the transmissivities varied from 1 to $1000 cm^2/sec$, which are typical values for the Gordo aquifer of Alabama and Mississippi. Rather than using these values, the parameters in the optimization problem were the log10 of these values.

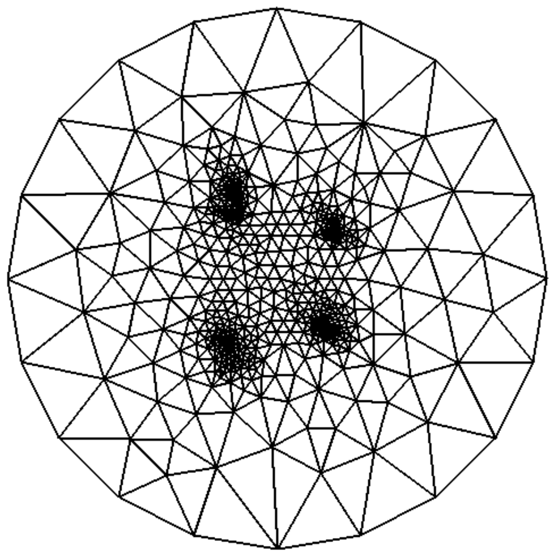

Figure 4. Unstructured Grid for Groundwater Modeling

The unsteady, optimization problem was tested on a computational grid consisting of 624 nodes and 1226 elements and had 4 pumping wells and 4 observation sights. This grid is given in Figure 4. Three different parameter grids were used to define the storage coefficient and transmissivity and consisted of 7 nodes, 13 nodes and 19 nodes. Two of these grids are shown in Figure 5.

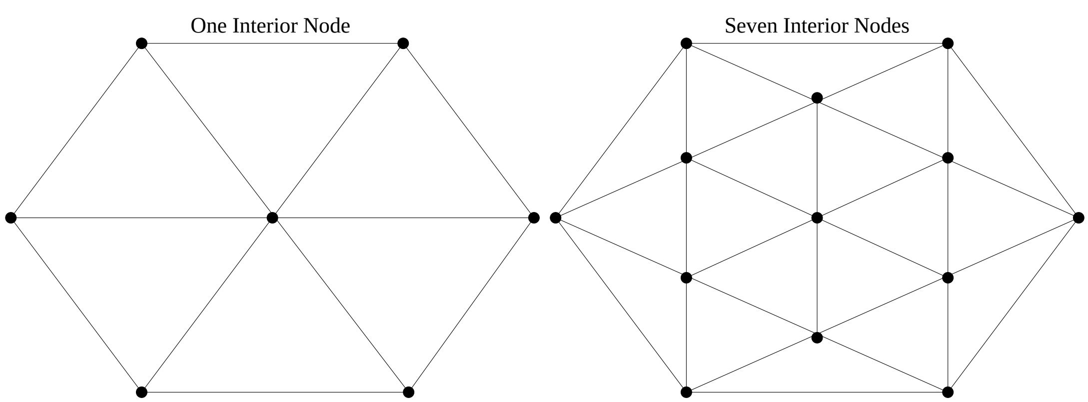

Figure 5. Parameter Grids of 7 and 13 Nodes.

The adjoint variable formulation was compared with the finite difference method for estimating gradients. The derivatives produced by both methods were in close agreement with each other as shown in Table 2. The results in Table 2 are for a parameter grid with 7 nodes, which is overly coarse. The first 7 parameter were the storage coefficients, and the final 7 parameters were the transmissivities. The adjoint variable formulation produces derivatives which are nearly identical to the more reliable finite difference derivatives, agreeing to approximately 6 significant digits.

Parameter	Adjoint Variable Formulation	Central Differences
1	-45925.025311358	-45924.992299115
2	-2287.0311627811	-2287.0295601024
3	-2660.9661401576	-2660.9633867338
4	-4127.9056919807	-4127.9018274508
5	-845.35360119004	-845.35319110728
6	-1832.6297783025	-1832.6283046918
7	-2975.3520004486	-2975.3513699688
8	-319348.54408843	-319348.57729211
9	-14375.214820738	-14375.216415647
10	-16081.800417180	-16081.803123961
11	-33795.079660431	-33795.083613950
12	-3385.7800768384	-3385.7803835417
13	-11656.581872462	-11656.583317381
14	-22342.723496048	-22342.724091141

Table 2. Comparison of Derivative Estimation Methods for 7 Node Grid.

The advantage of using the adjoint variable formulation, which is more difficult to implement than the finite difference approach, is the computational savings. In Table 3, the computational cost of estimating these sensitivities via the adjoint approach and the finite difference approach are presented for the 7, 13 and 19 node parameter grids.

Parameter Grid	Adjoint Variable Cost	Finite Difference Cost	Savings
7 Nodes	76.48	322.10	76.25 %
13 Nodes	117.43	600.21	80.44 %
19 Nodes	172.18	877.85	80.39 %
Comp. Grid	308.69	28830.4	1.071 %

Table 3. Comparison of Computational Costs of Estimating the Derivatives.

In order to demonstrate that this methodology actuals drives the parameters to the target values, the parameters are updated through several iterations via the inverse BFGS method. The optimization histories are given in Figure 6. The 7-node parameter grid is driven to machine zero in 65 iterations, when it achieves a function value of almost 10^{-20}. For the more complicated parameter grids, the optimal solution requires many more iterations.

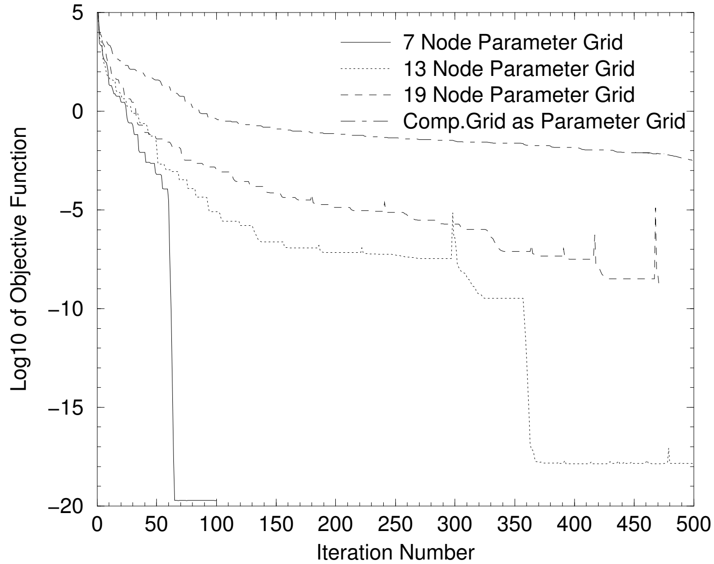

Figure 6. Optimization History for Groundwater Parameter Identification Problem.

Finally, the computational grid was used as the parameter grid, so that the value of the parameters at each node could be determined independently. The code was modified to take advantage of this structure, because only the elements associated with a particular node are directly dependent on the values of the parameters. As a result of this observation, the cost of evaluating the residual vector for the adjoint variable formulation greatly decreases. Once these modifications were made, the cost of evaluating a derivative via the adjoint variable formulation was less than 0.5 seconds, whereas for the previous problems, this cost was approximately 3.3 seconds. The derivatives generated in this fashion agreed with the finite difference derivatives to the same level of accuracy, and the optimization history is given in Figure 5. The objective function was not driven was reduced only 8 orders of magnitude after 500 iterations, as can be expected from the performance of the 19 node parameter grid; however, these initial results are encouraging. Better optimization algorithms are needed to update these design parameters more effectively.

7 Conclusions

In this paper, the adjoint variable formulation of discrete sensitivity analysis for both steady and unsteady problems has been presented. In this method, the adjoint variable is calculated through a tedious process, but once it has been determined, the cost of calculating the derivative of the objective function with respect to any parameter is quite small. For the problems presented herein, great computational savings is demonstrated for a steady-state design problem with 50 design parameters and an unsteady parameter identification problem with 624 parameters.

The steady-state problem dealt with the two-dimensional shallow water equations that were solved using a Petrov-Galerkin finite element code called HIVEL2D. The specific problem was to determine the optimal bed slope across a channel for a 90^o bend. Using the adjoint variable formulation to estimate the gradient in conjunction with the BFGS optimization algorithm, the optimal set of design parameters were found in 5 iterations. The derivatives compared well with the finite difference derivatives, agreeing to approximately 6 significant digits, whereas the computational cost of generating these 50 derivatives was only 4.75% the cost of using the complex Taylor's series expansion method.

For the unsteady problem, an unstructured, Galerkin finite element method was applied to the two-dimensional porous media equation to simulate flow in confined aquifers, with variable pumping rate wells and heterogeneous aquifer properties. Using the pumping rates and drawdown curves, an objective function that measured the difference between the observed and the computed drawdown curves was used. Initially, coarse parameter grids consisting of 7, 13, and 19 nodes were used to approximate the structure of the aquifer properties. In the last example, the value of these properties were determined for each node in the computational domain, which consisted of 624 nodes. The adjoint variable formulation was used to estimate these derivatives, which were in close agreement with the finite difference results. The inverse BFGS method was used to update these parameters, and the function value was decreased by 6 orders of magnitude.

As can be seen by these examples, the adjoint variable formulation of discrete sensitivity analysis generates derivatives that are accurate to approximately 6 significant digits and yet the computational cost is quite small for problems with large numbers of parameters. This gradient estimation method can be combined with the BFGS method to update the parameter values quite effectively, although as the number of design parameters grows, the performance of this algorithm is decreased.

8 References

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