Efficient Software for Computing K-Tomographs

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Abstract

A software has been developed in C++ for estimating hydraulic conductivity distribution in an aquifer using (1) FEM to model groundwater flow, (2) adjoint method to expedite sensitivity computation, and (3) statistical updating to incorporate observation data.

Motivation

A geological system is highly heterogeneous and uncertain. Subsurface contaminants tend to migrate through permeable zones. Reliable prediction of contaminant fate and transport hinges upon accurate delineation of the spatial distribution of hydraulic conductivity in the subsurface. A robust software is needed to facilitate the estimation of spatial distribution of hydraulic conductivity using aquifer test data.

FE Model

The differential equation governing steady-state groundwater flow is:

$$\nabla(K * \nabla h) = q$$

K: hydraulic conductivity tensor h: hydraulic head q: source/sink flux

The equation representing the FE solution can be expressed in matrix notation as follows:

$$[K] * \{h\} = \{q\}$$

Sensitivity Calculation

For estimating the updated parameters, we need to evaluate the sensitivites of the model response to the conductivities at each element. The sensitivities are obtained with the Adjoint Sensitivity Method. Let $g(\{p\})$ describe the system response at some specific node, where $\{p\} = log\{K\}$. The derivative of g in terms of each element $p_j$of $\{p\}$ is obtained through the following two steps ([1] and [2]):

1. Solution of the adjoint system:

$$[K](\{p\})\{\lambda_i\} = \frac{\partial {g_i}^T}{\partial\{h\}}$$

2. Evaluation of the sensitivity to each p_j in terms of the adjoint solution λ through vector-matrix multiplication. No additional solution of the system is needed:

$$\frac{\partial g(\{p\})}{\partial p_j} = \{\lambda_i\}^T \left(\frac{\partial\{q\}(\{p\})}{\partial p_j} - \frac{\partial[K](\{p\})}{\partial p_j}\{h\}(\{p\}) \right)$$

K-Estimation

The inverse problem of estimating the conductivities of the elements given observations $\{\hat{\mu}_{h,0}\}$ of the system response is solved employing a Bayesian approach [3]. The assumed prior mean vector $\mu_{p,prior}$ and covariance matrix $\Sigma_{p,prior}$ of $\{p\} = log\{K\}$ are updated following an iterative procedure. At each iteration a First Order Taylor Series expansion is performed at the current estimate of the updated mean. This requires the evaluation of the Jacobian $J = \frac{\partial g}{\partial p}$, where g denotes the model response at the location of the observations. The Jacobian is calculated with the Adjoint Sensitivity Method. The posterior mean and covariance are calculated through the following expressions:

$$\{\hat{\mu}_p\} = \{\mu_{p,prior}\} + [\Sigma_{ph}][\Sigma_{hh}^{-1}](\{\hat{\mu}_{h,0}\} - \{\mu_{h,prior}\})$$

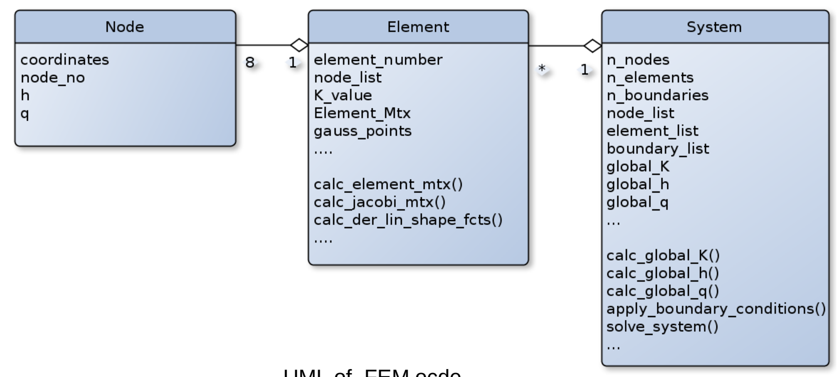
$$[\Sigma_p] = [\Sigma_{p,prior}] - [\Sigma_{ph}][\Sigma_{hh}]^{-1}[\Sigma_{hp}]$$

The unconditional covariance $[\Sigma_{hh}]$ and the conditional covariances $[\Sigma_{ph}]$ $[\Sigma_{hp}]$ are retrieved by multiplying the unconditional covariance $[\Sigma_{pp}]$ with the Jacobian as follows:

$$\begin{pmatrix} [\Sigma_{pp}] & [\Sigma_{ph}] \\ [\Sigma_{hp}] & [\Sigma_{hh}] \end{pmatrix} = \begin{pmatrix} [\Sigma_{pp}] & [\Sigma_{pp}]^T[J]^T \\ [J][\Sigma_{pp}] & [J][\Sigma_{pp}][J]^T \end{pmatrix}$$

Code Structure

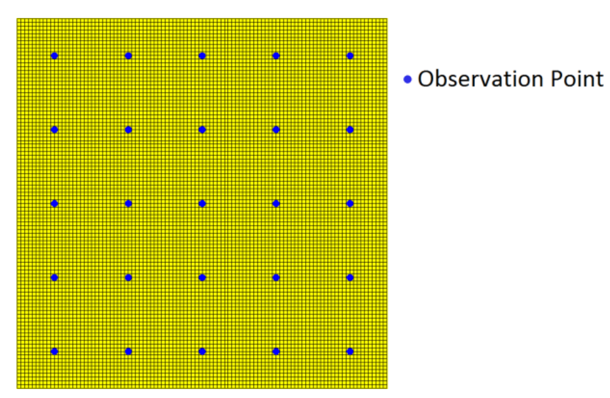
The FE-formulation is solved in an FE-program using an Conjugate Gradient solver from the library *Trilinos* [4]. The code structure is depicted in the UML diagram below.



UML of FEM ocde

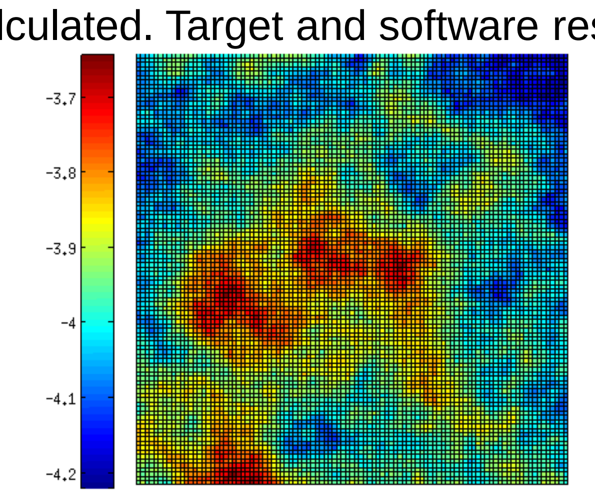
Computation Example

The model of an aquifer is represented by a uniform quadratic mesh with a length of 100 meters and a thickness of 1 meter. The elements are of size 1mx1mx1m. 25 observation point are evenly distributed over the domain. A natural groundwater flow is simulated by setting the hydraulic heads at one edge and the fluxes at the opposite edge of the domain.

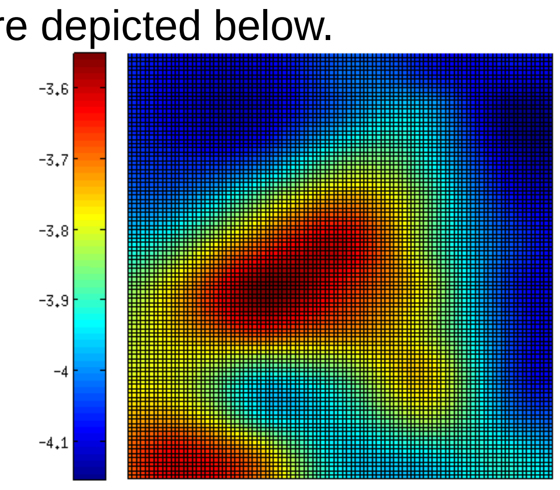


FE mesh side and plane view with location the observation points

For validation, a hydraulic conductivity distribution was created and back calculated. Target and software result are depicted below.



Simulated Target



Software result

Conclusions / Outlook

The usage of a Conjugate Gradient solver and a sparse matrix storage scheme allow modelling groundwater flow with the FEM program with highly refined meshes. The Adjoint Sensitivity Method provides the possibility to determine a large number of sensitivities, to form the Jacobian, with low computational effort. The inverse problem, i.e. the updating of the conductivities can therefore be executed precisely.

A further step would be the extension of the program with an integration of a time dependency.

References

[1] C.M. Mok: Conditional Reliability Analysis of Groundwater Flow and Subsurface Contaminant Transport, PhD Dissertation, University of California at Berkeley, 1999

[2] A.M. LaVenue and J.F. Pickens: Application of a coupled adjoint sensitivity and Kriging approach to calibrate a groundwater flow model, Water Resources Research, vol. 28, no. 6, pp. 1543-1569, 1992

[3] T.C. Jim Yeh and Shuyun Liu: Hydraulic Tomography - Development of a new aquifer test method, Water Resources Research, vol 36, issue 8, Aug 2000.

[4] Sandian National Laboratories: The Trilinos Project, url: www.trilinos.sandia.gov, 2013