# Numerical Modeling of Contaminant Transport in a Porous Medium; The Uncertainty in the Solution Arising from Uncertainty in Model Parameters.

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## 1 Introduction

Contaminant transport through a porous medium is described by the partial differential equation governing the conservation of mass. For multi-phase flow this relationship is given by

$$\phi \frac{\partial S_l}{\partial t} = -\nabla \cdot [K_l(\nabla P - \rho_l g)] + q_l \tag{1}$$

where $\phi$ is the porosity, $S_l$ is the volume fraction of phase $l$, $P_l$ is the pressure of phase $l$, $\rho_l$ is the density of phase $l$, $K_l$ is the permeability of phase $l$ within the medium, and $q_l$ is the volumetric production rate of phase $l$. This equation with the appropriate boundary conditions defines the three dimensional pressure field throughout a domain. Using Darcy's law the velocity field is then calculated using

$$V_l = -K_l(\nabla P_l - \rho_l g). \tag{2}$$

This field is then used in a conservation equation for the contaminant species that is suspended within this transporting fluid and concentration levels as a function of location and time are calculated.

The question posed in this workshop is; "What is the uncertainty in the resulting concentration levels given uncertainty in the model parameters?" The application of interest here is the transport of a contaminant species through geological structures. In this case, the largest uncertainty is in the parameter defining the local permeability $K_l$. Within geological structures this parameter can range from effectively zero in regions of clay, to very large values in regions of unimpeded flow through cracks and fissures. It is common that this range of permeabilities will be realized within the relatively small domains modeled by the numerical simulation. Finally, the "true" unknown permeabilities are often very poorly known.

We approach this problem by considering only single phase flow and developing ideas capable of describing the statistical behavior of the pressure field given the statistical behavior of the local permeabilities throughout the model domain. These techniques focus on the development of efficient Monte Carlo methods to derive a probability distribution for the pressure at a particular point. Given this distribution function,

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statements can then be made about the probability that the modeled pressure will be that which has been modeled.

We then approach the problem using techniques from linear sensitivity analysis. Using these techniques an efficient method for calculating the partial derivatives of the pressure with respect to each of the modeled permeabilities is derived. We then suggest ways in which these derivatives can be used with the Monte Carlo simulations to improve computational efficiency.

The pieces to be assembled and the assembly procedure for quantitative study of steady state single phase flow are;

(1) Input-1: geological information about the permeability throughout the domain of study. This includes observational data defining the permeability at specific locations throughout the domain, knowledge of the statistical distribution of the permeabilities within the domain, knowledge of the correlation length of the permeability field, and knowledge of geological features that influence the permeability field.

(2) Input-2: knowledge of the behavior of the pressure field on the boundaries of the domain of study required to define a unique solution to the partial differential equation.

(3) A geological model. A geological model transforms input-1 into a permeability field $K(x, y, z)$, defined at each grid point of the model. This model is described in more detail in Section (2).

(4) A numerical model solving the partial differential equation governing steady state single phase flow

The questions to be addressed here are the following:

(a) What is the pressure field, $P(x, y, z)$ for a particular realization of the permeability field $K$?

(b) What is the average pressure field, $< P(x, y, z) >$?

(c) What is the probability distribution of the pressure field?

Each of these questions asks for more and more detail about the connection between the permeability field, $K$, and the pressure field, $P$. Question (a) asks about one realization; it is answered by one run of the numerical model which solves equation (1). Question (b) is about an average that can be found by examining a reasonable number of realizations of $K$. Question (c) asks about the extreme statistics of the distribution of pressure field.

The real difficulty in answering the these questions is properly characterizing the relationship between the distribution of the permeabilities $K$ and that of the solution. The immense difficulty of this task can be illustrated with a simple calculation. Suppose one wishes to solve Equation (1) over a $1km \times 1km \times 1km$ volume. The permeability field has correlation length $10m$ over the entire volume. This means there are $\frac{1000m^3}{10m} = 10^6$ essentially independent volumes. Measurement of the permeability at 1000 points (each in a separate $10m \times 10m \times 10m$ block) reduces this number by a negligible amount. Roughly $10^6$ values of the permeability must be assigned from a reasonable model. If the permeability of each block took on at most two values, $K_1$ and $K_2$ there would be of order

$$2^{1000000} \tag{3}$$

independent, equally probable realizations. One can not examine even a tiny fraction of the total given the computational expense of one model run. In this work we examine methods that can be used to reduce the number of model runs which must be examined to produce accurate estimates of the distribution of the calculated pressure field.

# 2 Geological Modeling

## 2.1 Geostatistical Approach

In the previous section we discussed the need for a geological model of the permeability field (input 1). Typically these models are based on a geo-statistical approach which characterizes the permeability field $K(x, y, z)$ using a probability distribution function. In this case, $K$ at each point is assumed to be log normally distributed, and a function $C(h)$ defines the covariance between $K(x)$ and $K(x+h)$ [?]. The choice of the log normal distribution for $K$ is based on observations. The covariance function $C(h)$ is chosen to give the field realistic spatial structure. Although this approach is not completely satisfactory, it is reasonably realistic and mathematically tractable.

The next step in this approach is to produce a realization of the permeability field which is consistent with the limited number of observations of the permeability throughout the domain. This procedure is known the turning bands method. For a detailed description of this method see the work of Matheron [?].

## 2.2 Percolation Method

An alternative approach to modeling the effective permeability of a geological medium is the percolation method. The percolation recipe due to Ambegaokar et al. ([?] (several useful extensions have been made e.g. Katz and Thompson [?]).

There are physical arguments justifying the AHL recipe. We do not give them here but rather cite the empirical demonstration of its validity by Berman et. al. [?]. The original context for use of the AHL recipe was calculation of the electrical conductivity. Application of the recipe to the hydraulic permeability problem, follows from the correspondence between the electrical conductivity problem

$$\nabla \cdot \sigma \cdot \nabla V = 0, \tag{4}$$

(here $V$ is the voltage and $\sigma$ is the conductivity tensor) and the hydraulic conductivity problem

$$\nabla \cdot K \cdot \nabla P = 0, \tag{5}$$

$P \rightarrow V$ and $K \rightarrow \sigma$.

View the hydraulic system described by $K(\vec{x})$ as a network of hydraulic bonds. In order that the hydraulic bonds can be regarded as randomly distributed the bond length, spacing between nodes, of the lattice is taken to be of order the correlation length. The bond strengths are assigned according to any sensible rule that relates the pressure drop across a bond and resulting fluid current to the fluid flow properties of the volume $\xi^3$ the bond represents. Because the volumes $\xi^3$ are independent the bonds may be regarded a chosen from a distribution $p(K)$.

The procedure for estimating the hydraulic permeability of the network is:

(1) Remove all of the bonds keeping track of where they came from.

(2) Sort the bond according to strength, i.e. $K_1 > K_2 > \cdots$, where $1, 2, \cdots$ are the labels after sorting.

(3) Begin with $K_1$ and put the bonds back where they came from in the order (2). Continue this procedure until the resulting network of bonds percolates, i.e. spans the system (e.g. from left to right).

# 3 Monte Carlo Methods

In this section we investigate the use of Monte Carlo simulations to produce an estimate the probability distribution of the pressure at a fixed point in space. The pressure at a specific grid point is assumed to

be a random variable whose sample space is the set of permeabilities at each grid point throughout the model domain. We have assumed prior application of a geo-statistical model which defines the statistical distributions for each of these permeabilities.

The basic idea of the Monte Carlo method is to partition the sample space and to find the values of the random variable at the points in this partition. The values of the random variable are then weighted by the probabilities of each of the partition points, i.e. by the statistical representation of $K$. If one could partition the sample space finely enough, one could then get an accurate approximation of the random variable's distribution. As discussed in the introduction, the number of model runs required to completely sample the parameter space is prohibitively large.

An alternative tactic is to sample the $K$ values pseudo-randomly. This method can be understood by considering the evaluation of an integral using the Monte Carlo Method. Here, we estimate an integral over a very high dimensional domain by evaluating the integrand at randomly sampled points in the domain. If we were interested in only estimating the mean of our random variable, our problem would be identical to Monte Carlo integration, however we wish to know the entire distribution and in particular its tail. In this case we are again faced with the difficulty of the very high dimensionality of the sample space leading to extreme computational time required to accurately characterize the entire distribution.

The major drawback of Monte Carlo methods is that with a pseudo-random sampling of data, one is unlikely to generate sets of data that are evenly distributed. This problem has been the motivation for developing quasi-random number generators. Quasi-random sequences are deterministic (two sequences using the same generator are identical), but they guarantee that the sequence of numbers generated will be distributed throughout the parameter space without losing any statistical properties. One of the simplest quasi-random generators is called the Halton sequence [?] [?] [?]. Given a prime number $p$, this sequence generates a sequence of numbers in the interval $[0, 1]$ using fractional representations based on the sequence $\{ \ldots \}$. Each dimension of the system uses a different base number $p$ to generate a sequence. Choosing the bases of the sequence to be prime numbers ensures that sequences for different components of the parameter space will not correlate with each other. The convergence rate for problems using these generators has been shown to be

$$\frac{(\log N)^s}{N}$$

where $s$ is the dimension of the system and $N$ is the number of samples.

Because the primary problem is the extreme computational expense of repeated Monte Carlo simulations, any reduction in the dimensions of the sample space will speed up the computations and perhaps allow for methods with better convergence. For example, if large regions are of a homogeneous material or contain man-made structures, the permeabilities will be known reasonably well and do not have to be treated statistically. Also, large features such as sand bars, bodies of water, and faults can be modeled as single random variables.

# 4 Parameter Fitting Methods

Parameter fitting methods assume that the pressure at each grid point has a known distribution which is a function of a limited number a parameters. For example in the simplest case one might assume that the pressure is distributed log normally and the problem is reduced to finding a mean and a standard deviation. In this section we investigate the utility of implementing these methods for the problem studied here.

The first method considered is the moment method. In this case, the mean and variance of the permeability field, $K$, are assumed to be known at each point. We then construct a Taylor series approximation

to $P(K)$, expanding around the mean conductivity field $\bar{K}$.

$$P(K) = P(\bar{K}) + \nabla P(\bar{K})(K - \bar{K}) + \dots$$

If we drop all higher order terms and take the expected value of both sides, we obtain the estimate

$$E[P(K)] = P(\bar{K}).$$

Similarly, we can obtain an estimate of the variance of $P(K)$

$$E[(P(K) - P(\bar{K}))^2] = E[(\nabla P(\bar{K})(K - \bar{K}))^2]$$

This estimate requires only knowledge of the covariance structure of $K$, $P(\bar{K})$ and its first and second derivatives.

A second approach is suggested by the perturbation formulation of the problem, developed by P.R. King in his 1987 paper "The Use of Field Theoretic Methods for the Study of Flow in heterogeneous Porous Medium". To develop his method, he assumes that the system is homogeneously anisotropic, i.e. only one coordinate transformation is needed to diagonalize the permeability tensor. He defines the Green's function for the partial differential equation by

$$\nabla_r \cdot K(r)\nabla_r G(r, r') = \delta(r - r') \tag{6}$$

and uses the permanent flux condition to get:

$$p(r) = q \cdot \int G(r, r')dS. \tag{7}$$

If we consider perturbations about the permeability $K_0$ of a homogeneous medium,i.e.

$$K(r) = K_0 + y(r) \tag{8}$$

then the Green's function for the perturbed problem is given by

$$K_0 \nabla G = \delta(r - r') - \nabla \cdot y \nabla G. \tag{9}$$

Taking the inverse of both sides, converting the differential equation into an integral equation and taking the Fourier transform, gives us an iterative scheme for finding the perturbed Green's function.

$$G(j, k) = G_0(j)\delta(j + k) + G_0(j) \int K_0[(l + m) \cdot m]\delta(l + m - j)y(l)G(m, k)dldlm \tag{10}$$

King uses diagrammatic representation to develop the Green's function as a perturbation expansion series, which could be averaged term by term. To determine the n-th term in this series, it is necessary to determine the moments of the perturbation $y(r)$. As mentioned above, a log-normal distribution is assumed for the permeability tensor.

$$P[K(r)] \sim exp(-\frac{1}{2} \int \int ln\frac{K(r)}{K_g} \rho^{-1}(r - r') ln\frac{K(r')}{K_g} drdr' \tag{11}$$

If the variance is small in comparison with the mean, a Gaussian approximation may be used for the moments of the permeability fluctuations. The author uses the methods of field theory, and more specifically diagrammatic representation to derive the perturbation expansion for an "average" Green's function. This is done in much detail in King's paper. From now on we will be dealing with the so called effective permeability, which gives us the mean behavior of a heterogeneous medium. The effective permeability could be calculated

and the result is $K_{eff} = K_0(1 - \rho(0)/d)$, where $d$ is the spatial dimension. If we decide to use Gaussian approximation, the above expression is the first-order approximation to an exponential:

$$K_{eff} = K_0(-\rho(0)/d) = K_g exp[\rho(0)(\frac{1}{2} - \frac{1}{d}]. \tag{12}$$

In comparison with previous results in the literature this one is more general because it does not bear any restrictions by the space dimension. It turns out that for dimensions higher than 1, the geometric mean is the correct effective permeability. It is either exact (2 dimensions) or leads to a very close approximation(3 dimensions). These conclusions are based on extensive numerical calculations.

Using the effective permeability and the average (re-normalized) Green's function, we may calculate the mean fluid pressure in the medium:

$$p(r) = \frac{q}{K_{eff}} \cdot \int \mid r - r' \mid^{2-d} dS' \tag{13}$$

Some justification for the use of perturbation theory is needed for each physical problem, since they could be highly individual. Also, the Gaussian distribution is not always a valid approximation for the log normal distribution, so there is some loss of accuracy, as well. In the process of deriving the above results, the author assumes that the correlations die away quickly for large distances and hence he feels justified to keep only terms of [illegible] series (for more detailed information, see the original paper). Another parameter for each random variable is its variance. For the pressure, it is defined as:

$$\sigma_p^2(r_1, r_2) = < p(r_1)p(r_2) > - < p(r_1) >< p(r_2) = \int \{ \quad (r_1, r_1')G(r_2, r_2') > - < G(r_1, r_1') >< < G(r_2, r_2') > \} dS_1 dS_2' \tag{14}$$

assuming that the system is statistically homogeneous, so that the pressure variance can only depend on $r_1 - r_2$ and again heavily using diagrammatic methods, the author reaches to the following result:

$$\sigma_p^2 = \frac{q^2 exp(2\rho(0)\backslash d)}{dK_{eff}^2} \rho(0)\lambda^2 S_d \tag{15}$$

where $S_d$ is some general geometric factor, which depends on the shape of the boundary through which the flow takes place.

We could see from the above exposition that even calculating the first two moments for the pressure field presents big conceptual and computational problems. To make things worse, knowing only the mean and the variance is not good enough to get a good idea about the shape of the pressure distribution. We need at least two more moments and the method, suggested by King becomes impossible to carry out.

A different approach is to assume that the pressure distribution could be fitted by parametric family of distributions, such as the Generalized Lambda or Beta Family of Distributions. Because of their generality (both families possess 4 free parameters, which allow some degrees of freedom), they are known to cover all of the known distributions. The idea is to match some sample characteristics (like moments or percentiles) to the distribution ones, solve a system of equations for the parameters and build a theoretical distribution, from which we could sample. The problem of finding more than the first two sample moments was discussed above. The idea of using percentiles instead of moments is tempting and works quite well for simpler problems. However, to build sample percentiles and to decide which ones characterize the shape of the pressure distribution, we need to run a lot of simulations, i.e. that brings back to the problem we are trying to solve. Unfortunately, while the 50th percentile, or the median, often comes close to the mean, a similar parallel is missing for any other percentile and so that idea had to be dropped.//

# 5 Numerical Results

Numerical tests were performed to gain insight into the strengths and limitations of the Monte Carlo simulation and the method of moments for approximating the mean and variance of the pressure given a statistical model for the permeability field. The simulations were based on the two dimensional pressure equation

$$\begin{aligned} \nabla \cdot (K \nabla \mathbf{P}) &= 0 \quad \text{in } \Omega, \\ \mathbf{P} &= G \quad \text{on } \delta\Omega \end{aligned} \tag{16}$$

where $\Omega$ is the unit square, $\delta\Omega$ the boundary of $\Omega$ and $K$ the $2 \times 2$ diagonal conductivity matrix. The second order finite volume discretization approximation to Equation (6) was defined on a cell–centered $nXn$ grid as depicted in Figure 1, where average values of K are defined at the grid centers (grid points). The five–point finite difference equation is defined at the interior points by

$$\nabla \cdot (K \nabla \mathbf{P})_{i,j} \approx \frac{1}{h^2}(K_{i-\frac{1}{2},j} P_{i-1,j} + K_{i+\frac{1}{2},j} P_{i+1,j} + K_{i,j-\frac{1}{2}} P_{i,j-1} + K_{i,j+\frac{1}{2}} P_{i,j+1} + C_{i,j} P_{i,j}) \tag{17}$$

where the diagonal coefficient, $C_{i,j}$, is the negative sum of the other coefficients and the off–diagonal coefficients are defined by harmonic averaging, i.e.

$$K_{i\pm\frac{1}{2},j} = \frac{1}{\frac{1}{2}\left(\frac{1}{K_{i,j}} + \frac{1}{K_{i\pm1,j}}\right)}.$$

The Dirichlet conditions at the boundaries are approximated by linear averaging of $U$ between the ghost points and their adjoining interior points.

A simulation consisted of first generating N log normally distributed correlated permeability fields, $K$, with a given correlation distance. The finite volume equations were solved for the corresponding pressures. The mean and variance of the pressures at selected points were then calculated and compared with the mean pressure field $\bar{P}$ calculated from the mean conductivity field $\bar{K}$ and the standard deviation computed by the method of moments, respectively.

For predicting the variance of the pressure, the Jacobian matrix, $dP/dK$, evaluated at the mean permeability field $\bar{K}$ was calculated using forward differences. Specifically, for each $i$ and $j$ in the computational grid, the perturbed pressure $\tilde{P^{i,j}}$ was calculated from the perturbed permeability field $\tilde{K}$ where $\tilde{K}_{i,j} \leftarrow \bar{K}_{i,j} + .001$. The corresponding entries of the Jacobian are approximated by

$$\left.\frac{dP^{i,j}}{d\tilde{K}}\right|_{x,y} \approx J = \frac{\bar{P}_{x,y} - \bar{P}^{i,j}_{x,y}}{.001}. \tag{18}$$

The variances of $P$ that are predicted by the method of moments are then obtained from the corresponding diagonal entries in the matrix $J(dP/dK)J^T$.

Our first test was conducted on a 10X10 grid (cell size = .1) with the mean, variance and correlation length of the permeability fields given by 10, 60 and .3, respectively. The boundary conditions were defined with G(x,y) equal to 1 at $(0,0)$, 2 at $(0,1)$, 1 at $(1,1)$ and 4 at $(1,0)$ and linear between these points along the boundaries. The resulting pressure statistics were measured near the center and near the sides of the domain. The computed mean of $P$ at the selected points agreed with those of $\bar{P}$ to two decimal places whereas the predicted variances were significantly off. However, when we reduced the variance of $K$ to 6, we got good (2 or 3 digit) moment method estimates of both the mean and standard deviation of the pressure. Thus the moment method works reasonably well for estimating the variance of $P$ when the variance of $K$ is small, but the method breaks down as the variance of $K$ gets larger. For estimates of the average pressure, the moment method is somewhat more robust. This isn't unexpected, but it tells me that the moment method may not be appropriate for real world problems with significant uncertainties in $K$.

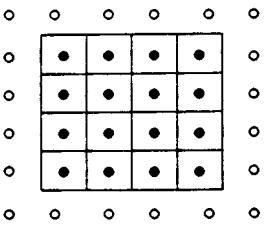

Figure 1: Typical two–dimensional cell–centered computational grid. Interior points are indicated by • and ghost points by ∘.

# 6 Variational Methods

The problem of finding the pressure field, $P(x, y, z)$, that satisfies the steady state single phase flow equation has a variational formulation. This formulation is particularly advantageous because the variational functional is the average permeability. In this section we describe the derivation of the variational principle and discuss ways in which it can be useful.

(a) The Variational Functional.

The equation

$$\nabla \cdot K \cdot \nabla P(\vec{x}) = 0, \tag{19}$$

is to be solved for the pressure field in the domain $D$ subject to the boundary conditions $P(x = 0, y, z) = P(0)$ and $P(x = L, y, z) = P(L)$. The velocity field at $\vec{x}$ is found from

$$\vec{v}(\vec{x}) = -K \cdot \nabla P(\vec{x}). \tag{20}$$

The average permeability, $\overline{K}$, is defined in terms of the average velocity field;

$$\overline{v}_x = \frac{1}{A} \int dy\, dz\, \hat{e}_x \cdot \vec{v}(\vec{x}) \equiv -\overline{K} \frac{P(L) - P(0)}{L}, \tag{21}$$

. The variational equation for $\overline{K}$ is found starting from

$$\nabla \cdot [P(K \cdot \nabla P)] = \nabla P \cdot K \cdot \nabla P + P \nabla \cdot [K \cdot \nabla P]. \tag{22}$$

This equation is integrated over $D$. The second term on the right hand side is zero from Equation (17). The left hand side of the equation is transformed to a surface integral using Gauss's theorem, the resulting surface integral is evaluated using the equation for the velocity field and the definition of $\overline{K}$ with the result

$$\int d\vec{x}\, \nabla \cdot [P(K \cdot \nabla P)] = \overline{K} \frac{A}{L} (P(L) - P(0))^2. \tag{23}$$

Thus

$$\overline{K}[P] = \frac{\int d\vec{x}\, \nabla P \cdot K \cdot \nabla P}{\left(\frac{P(L) - P(0)}{L}\right)^2}. \tag{24}$$

(b) Uses of the variational principle.

(i) The equation for the pressure field, (17), is found by varying $\overline{K}[P]$ with respect to the function $P$. [A point of pedagogic value.]

(ii) The pressure field can be found as the function $P$ that minimizes $\overline{K}[P]$ This fact can be used to computational advantage, see (iv).

(iii) $\overline{K}$ is stationary with respect to small changes in $P$. As a consequence the change in the permeability that results from change in $K$ can be found approximately as

$$\overline{K}_\mu \approx \int d\vec{x}\, \nabla P_\nu \cdot K_\mu \cdot \nabla P_\nu \tag{25}$$

where

$$\overline{K}_\nu = \int d\vec{x}\, \nabla P_\nu \cdot K_\nu \cdot \nabla P_\nu. \tag{26}$$

(iv) An upper bound on $\overline{K}$ can be found using plausible guesses for $P$.

The variational principle should prove useful for answering questions that relate to the average permeability of a flow field. Unfortunately there are no equivalent formulations of calculation of $P(\vec{x})$ or $\vec{v}(\vec{x})$.

**Remark**

If we seek $P(\vec{x})$ appropriate to a particular realization of the permeability, we can find $P(\vec{x})$ exactly by implementing the computation called for by Equation (1). The numerical procedure transforms $K$ into $P(\vec{x})$. Denote this $P(\vec{x})$ by $P_\nu(\vec{x}) = T[K_\nu]$ or simply $P = T[K]$. It takes about 10 minutes to perform one transformation, $P = T[K]$. It takes about one week to perform a thousand transformations. Can we find a more economical way to proceed.?

Suppose we have $N$ realizations of $K$ in hand. We want to answer the question: what is the probability that the pressure at $\vec{x}$ is less that $P_0$? This can be restated as: for what fraction of the $N$ realizations is $P(\vec{x}) < P_0$? Suppose that for a few of the realizations of $K$ we carry through the transformation $T[K]$. For realization $\nu$ we find $P_\nu(\vec{x}) < P_0$. Suppose also we have a measure of the "distance between realizations", $d_{\nu\mu}$. When $d_{\nu\mu}$ is small compared to 1 realizations $K_\nu$ and $K_\mu$ are near one another and $P_\nu = T[K_\nu]$ and $P_\mu = T[K_\mu]$ are near one another. If we know $d_{\nu,\mu}$ for the N realizations we can sort them according to $d_{\nu,\mu}$ and obtain an approximate estimate of how many realizations are near $K_\nu$ or equivalently what fraction of realizations give $P(\vec{x})$ near $P_\nu(\vec{x}) < P_0$. We could further refine this sorting by judicious implementation of the transformation T[K]. Assuming that the time required to compute the distance measure, $d_{\nu,\mu}$ , is modest, we would have a great economy of time.

Is this pie in the sky or is it a practical procedure? A number of possible realization distance measures can be constructed. For example

$$d_{\nu,\mu} = \sum \left[ \frac{K_\mu(i)}{|K_\mu|} - \frac{K_\nu(i)}{|K_\nu|} \right]^2 \tag{27}$$

The basic physical process taking place in the system is fluid flow. Two realizations that lead to much the same velocity field would be judged to be near one another. The distance measure in Equation.(11) has no special sensitivity to the velocity field associated with the realizations.

A simple estimate of the velocity field associated with a realization of the permeability is provided by the percolation recipe for identifying the critical (percolation) path. A distance measure that compared the critical path of two realizations might prove to be effective in permitting a useful sorting of realizations. Work on an idea along these lines should be undertaken.

# 7 Linear Sensitivity Analysis

Linear sensitivity analysis of modeled physical systems is based on the analysis of the partial derivatives of the modeled response with respect to the modeled parameters. These derivatives can be used to identify the most important modeled parameters and can be used to estimate the uncertainty in the modeled response

arising from uncertainty in the modeled parameters. Here we investigate the feasibility of applying adjoint techniques to calculate these derivatives. For general discussion of these methods see the work of Cacuci [?] [?]. For application of these ideas to problems in geophysics [?] [?]. At the end of this discussion an alternative technique developed by computer scientists, automatic differentiation will be briefly discussed and references of detailed discussions and applications will be outlined.

To illustrate the formulation of the general adjoint equations we present a derivation applicable to a general set of non-linear partial differential equations. Consider a general set of nonlinear, coupled differential equations, the associated initial conditions, and a model response.

$$\frac{du_i}{dt} = f_i(\vec{u}, \vec{\alpha}, t) \tag{28}$$

$$\vec{u}(0) = \vec{\beta} \tag{29}$$

$$R(\vec{u}, \vec{\alpha}) = \int_0^{t_0} r(\vec{u}, \vec{\alpha}, t)dt. \tag{30}$$

Here $\vec{u}$, $\vec{\alpha}$, and $\vec{\beta}$ denote vectors of dependent variables, model parameters and initial conditions, respectively, and R denotes a general model response that is to be evaluated by the user. The operator $f$ is a general non-linear operator which may contain spatial derivatives in which case appropriate boundary conditions must also be imposed. The perturbation equations associated with each of these equation are written as

$$\frac{d\delta u_i}{dt} = \nabla_u f_i \cdot \delta\vec{u} + \nabla_\alpha f_i \cdot \delta\vec{\alpha} \tag{31}$$

$$\delta\vec{u}(0) = \delta\vec{\beta} \tag{32}$$

$$\delta R = \int_0^{t_0} \nabla_u r \cdot \delta\vec{u}dt + \int_0^{t_0} \nabla_\alpha \cdot \delta\vec{\alpha}dt. \tag{33}$$

Here $\delta\vec{u}$, $\delta\vec{\alpha}$ and $\delta\vec{\beta}$ denote small perturbations in the dependent variables, the model parameters, and the initial conditions, respectively, and $\nabla_u$ and $\nabla_\alpha$ denote gradient operators acting with respect to the dependent variables and the parameters. Using the direct method the perturbation in the response $\delta R$ is obtained by solving Equations (29) and (30) and imposing a specific parameter perturbation $\delta\vec{\alpha}$. The resulting $\delta\vec{u}$ is then used in Equation (31) to obtain $\delta R$. In practice since the number of linearly independent choices of $\delta\vec{\alpha}$ is equal to the number of parameters a complete sensitivity analysis would require solving equations (29) and (30) repeat-ably for each independent parameter. As discussed throughout this work the extreme size of the parameter space for the problem studied here prohibits this calculation.

The adjoint method eliminates this computational expense. In matrix notation equation (29) can be rewritten as

$$\mathbf{L}\delta\vec{u} = \mathbf{Q}\delta\vec{\alpha} \tag{34}$$

$$L_{ij} \equiv \delta_{i,j}d/dt - \partial f_i/\partial u_j \tag{35}$$

$$Q_{i,k} \equiv \partial f_i/\partial \alpha_k. \tag{36}$$

The adjoint to the operator $\mathbf{L}$ is defined by the relationship

$$\int_0^{t_0} \mathbf{L}^\dagger\vec{v} \cdot \delta\vec{u}dt = \int_0^{t_0} \mathbf{L}\delta\vec{u} \cdot \vec{v}dt - [\vec{v} \cdot \delta\vec{u}]_0^{t_0}. \tag{37}$$

Identifying $\mathbf{L}^\dagger\vec{v}$ in Equation (35) with $\nabla_u r$ and requiring $\vec{v}$ to satisfy the following conditions,

$$\mathbf{L}^\dagger\vec{v} = \nabla_u r \tag{38}$$

$$\vec{v}(t_0) = 0, \tag{39}$$

Equation (31) becomes

$$\delta R = \int_0^{t_o} \mathbf{Q}\delta\vec{\alpha} \cdot \vec{v}dt + \vec{v}(0) \cdot \delta\vec{u}(0) + \int_0^{t_o} \nabla_\alpha \cdot \delta\vec{\alpha}dt. \tag{40}$$

Noting that the elements of the second term are known from the initial conditions of the forward problem and the solution to the adjoint problem, all dependences in Equation (31) on all unknown elements of $\delta\vec{u}$ have been eliminated. Therefore, by solving the adjoint Equations, (36) and (37), once for $\vec{v}$, a complete sensitivity analysis for small perturbations in the parameters can be obtained by computing $\delta R$ using Equation (38) for each parameter.

In summary, the motivation for formulating the adjoint problem is to eliminate all dependencies in Equation (31) on the perturbation in the dependent variables, eliminating the need to rerun the forward model for each parameter. Note that an essential feature of this derivation is the expression of the response as an integral. The expression given by Equation (28) is sufficiently general to include most responses of interest. For example in the problem studied here the response of interest is is the pressure at a specified spatial and temporal coordinate which can be expressed in integral form as

$$P(\vec{r'}, t') = \int_V \int_0^T P(\vec{r}, t)\delta(t - t', r - r')dtdV. \tag{41}$$

The actual derivation of the adjoint operator requires first writing the complete perturbation equation, multiplying each term by the adjoint variable $v$ and then integrating the term involving perturbations in the model response by parts until the adjoint relationship is satisfied. To illustrate this derivation and to show the particularly useful result that for steady state flow through a porous medium the operator is "self-adjoint" we apply these methods to the partial differential equation for single phase steady flow as defined by

$$\nabla \cdot [K\nabla P] = q. \tag{42}$$

This equation with associated boundary conditions defines the pressure throughout the spatial domain. The response of interest is defined to be the pressure at a specified spatial coordinate and is given by the expression

$$P(r_\prime) = \int_V \delta(\vec{r} - \vec{r'})P(r)DV. \tag{43}$$

The first variation of this response to arbitrary perturbation in the model parameters is

$$\delta R = \int_V \delta(\vec{r} - \vec{r'})\delta PDV. \tag{44}$$

This variation is also defined by substituting $P = P + \delta P$ and $K = K + \delta K$ into equation (40) and obtaining

$$\nabla \cdot [\delta K\nabla P] + \nabla \cdot [K\nabla\delta P] = 0 \tag{45}$$

Here the first order terms cancel and terms that are quadratic in the perturbations have been neglected. Multiplying Equation (43) by an arbitrary function $v$ and integrating over the domain yields

$$\int_V v\nabla \cdot [\delta K\nabla P]dV + \int_V \delta P\nabla \cdot [K\nabla v]dV + vK\nabla P|_\Omega - \delta PK\nabla v|_\Omega = 0 \tag{46}$$

Here the last two terms result from integrating the second term in Equation (43) by parts twice and the subscript $\Omega$ denotes evaluation on the boundary. Observing that the second term in Equation (44) will be equal to the right hand side of Equation (42) if we require

$$\nabla \cdot [K\nabla v] = \delta(\vec{r} - \vec{r}_\prime) \tag{47}$$

and making the appropriate substitutions, the first variation in the response is expressed as

$$\delta R = -\int_V v\nabla \cdot [\delta K \nabla P] dV - vK\nabla P|_\Omega + \delta P K \nabla v|_\Omega \tag{48}$$

Note, that as in the derivation for the general case the boundary terms obtained by integrating by parts can be forced to vanish by imposing boundary conditions on $v$. Note also that Equation (46) is independent of $\delta P$ and therefore once $v$ is calculated the change in the response due to a change in an arbitrary perturbation in the parameters $K$ can be calculated by simply integrating equation (46). In many cases the partial differential equation governing the adjoint equations is different from that governing the original partial differential equation. The important result here is that these partial differential equation are identical (i.e. the differential operator is self adjoint) and therefore the original numerical model can be used to calculated the solution to the adjoint equations, eliminating the need to write a complicated numerical model for the adjoint equations. A similar result can be derived for the full multi-phase problem.

This derivation has shown that the partial derivatives of the pressure at a specific spatial and temporal coordinates with respect to each permeability defined within each grid space of the model can be calculated with an approximate computational expense equal to one model simulation. Although this is a useful result, this calculation will yield only linear sensitivities valid only for small perturbations.

A contrasting approach to developing sensitivity enhanced numerical simulation models is being pursued by computer scientists designing "pre-compilers". These pre-compilers are designed to automatically produce a modified code that includes a calculation of the partial derivatives given only the fortran or C code of the original model. This approach called automatic differentiation is based on the repeated application of the chain rule on a series of unary and binary operations. Automatic differentiation is performed by considering the solution to be a series of either unary or binary algebraic operations. Each operation is then differentiated with respect to the final solution using the chain rule and an expression for the partial derivatives of the solution with respect to each parameter is calculated.

Some advantages of this approach include a massive reduction in the man hours required by the adjoint method to produce the sensitivity enhanced model code, a large reduction in the probability of errors occurring during in the process of producing the sensitivity model code, the elimination of the need for two codes to be maintained together, a reduction in the memory required to calculate the adjoint variables and finally a reduction in cancellation and truncation error since the derivative calculation is exact. Furthermore, the developers of these pre-compilers continue active research into the continued enhancement of these tools promising, among other things, the ability to calculate second order derivatives and the parallelization of the calculations. For a thorough discussion of the theory, application and implementation of this method see the work of Greiwank [?]. Leading the development of these tools is the pre-compiler ADIFOR, developed in the combined works of [?] (1992). Finally for a discussion of the specific application of this method to ground water transport model see the work of [?]

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