PERCOLATION-BASED TECHNIQUES FOR UPSCALING THE
HYDRAULIC CONDUCTIVITY OF SEMI-REALISTIC
GEOLOGICAL MEDIA

A thesis submitted in partial fulfillment
of the requirements for the degree of
Master of Science

By

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Abstract

Idriss, Bilal. M.S., Department of Earth and Environmental Science, Wright State University, 2008. Percolation-Based Techniques for Upscaling the Hydraulic Conductivity of Semi-Realistic Geologic Media

I tested three schemes for “upscaling” the hydraulic conductivity (K) on aquifers with bimodal K distributions. This bimodality (e.g., sand and mud deposits) was intended to capture typical geological conditions. Results were tested with a numerical model. Upscaling techniques used were inspired by schemes interpolating between arithmetic and harmonic means, but are based on percolation theory: 1) Critical path analysis (CPA), 2) Percolation path analysis (PPA, or standard scaling), and a novel scaling approach. Models chosen were both spatially correlated and uncorrelated, with important differences in critical percolation probabilities, Pc. Volume fractions Ps and 1-Ps (with Ps = sand volume fraction) were assigned to each mode of the distribution of K. I found that application of the requirement for CPA to interpolate smoothly between the parallel and series configurations makes it satisfactory only for Ps>Pc. PPA generally underestimates K. The novel scaling technique has the widest generality.
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Dedication

“I dedicate the thesis to my parents for their continuous support...”
I. Introduction:

Verifiable prediction of the effective hydraulic conductivity is needed in any field that requires discrete characterization of an aquifer, because of the difference in scale at which measurements are taken from the field and the numerical solution for flow (Wen and Gomez-Hernandez, 1996). When such prediction of effective properties proceeds from knowledge of their variability at smaller spatial scales this technique is referred to as upscaling. The successful application of upscaling requires understanding of both upscaling theory and the impacts of heterogeneity on $W(K)$ on input scales. I will discuss both of these topics in this thesis, but the emphasis will be on the upscaling techniques.

Consider an aquifer composed of two facies or strata. Assume that the statistical and geometrical properties of each facies or stratum are known. Would it be possible to estimate/calculate the hydraulic conductivity of the aquifer without representing the aquifer with a computer simulation? The thesis at hand studies three methods for the “upscaling” of the hydraulic conductivity of two distributions based on percolation theory.

Upscaling of the hydraulic conductivity ($K$) is a mathematical procedure to find an effective value of $K$ for a medium for which one knows the variability of $K$ at smaller scales.
Such variability is normally expressed as a probability density function, $W(K)$ in the variable $K$. Thus a complete understanding of upscaling must encompass the ability to predict a distribution of $K$ values from knowledge of that distribution at smaller scales (Hunt, 1998). In this thesis prediction of a full distribution of $W(K)$ at larger scales will not be attempted, and only a most likely $K$ value will be found. The most likely value of $K$ will be equivalent to the ensemble mean value of $K$ only in the limit of infinite size as, because finite-size corrections generate systematic deviations from the infinite size result (Hunt, 2001a).

Upscaling in the geology domain is needed for hydrology, the oil industry, and in hydrogeology. These applications include: in hydrology; sequestration of carbon dioxide, and monitoring and remediation of spills, in the oil industry; understanding of extraction as well as migration of hydrocarbons, in hydrogeology; understanding the behavior of sedimentation, diagenesis, and other processes involving fluid flow

Physicists have developed a number of methods to solve such problems, such as percolation theory, perturbation theory, effective-medium theory and stochastic homogenization (among others). The first is a suitable technique for distributions with large variance (Seager and Pike, 1974), the second is generally restricted to systems with small variance in $W(K)$, while the third method can perform reasonably well at all variances. In some cases, percolation theory can also be formulated to produce accurate solutions that
interpolate smoothly between cases with small and large variances (Bernabe and Bruderer, 1998, for example). This particular thesis in fact is based on such an attempt.

Geologists and hydrologists also have a collection of descriptions for upscaling the hydraulic conductivity, such as those described in Matheron (1963), De Wit (1995), and Scheibe and Yabusaki (1998). These methods can also be discussed in standard physics terms. As pointed out in De Wit (1995), the Matheron result (1963) can be regarded as a truncated perturbation expansion. A perturbation expansion can only converge when the perturbation parameter is small. As pointed out by Hunt, 2008, the treatment presented in Scheibe and Yabusaki (1998) (described in the next paragraph) is merely an interpolation, without physical basis. I will show, however, that this interpolation can help inspire a more physically-based interpolation scheme.

The effective hydraulic conductivity of any distribution, whether mono-modal or multi-modal, must clearly fall between its harmonic and arithmetic mean values, since these correspond respectively to configuring all the individual K’s either in series or in parallel. However, building a mathematical model to incorporate this physics has proved difficult. Consider a model presented in Scheibe and Yabusaki (1998).
Equation 1

\[
K_{\text{eff}} = \left[ \frac{\int_{K_{\text{min}}}^{K_{\text{max}}} K^{-\mu} W(K) dK}{\int_{K_{\text{min}}}^{K_{\text{max}}} W(K) dK} \right]^{1/\mu}
\]

In equation 1 when \( W(K) \) is appropriately normalized the denominator will be equal to one. The hydraulic conductivity that the model generates falls between the harmonic mean (when \( \mu = -1 \)) or the arithmetic mean (when \( \mu = 1 \)), and yields in particular the geometric mean when \( \mu \) approaches zero (Scheibe and Yabusaki, 1998). Accordingly any possible upscaled effective hydraulic conductivity can be developed for some value of \( \mu \). It is important that choice of any value of \( \mu > 0 \) (\( \mu < 0 \)) maximizes the importance of the largest (smallest) \( K \) in the distribution.

Perturbation theory generates the following expression for the effective hydraulic conductivity of a medium with small variance, \( \sigma^2(K) \) (Gutjahr et al., 1978; Dagan, 1979;

Equation 2

\[
K_{\text{eff}} = K_{\text{GM}} \left[ 1 + \left( \frac{1}{2} - \frac{1}{m} \right) \sigma^2(K) \right]
\]
with $m$ the spatial dimensionality of the system and $K_{GM}$ the geometric mean of the distribution. If one takes advantage of the expansion $\exp(x) = 1 + x$ to lowest order in $x$, this perturbation expression can also be written in the form

**Equation 3**

$$K_{\text{eff}} = K_{GM} \exp\left[\left(\frac{1}{2} - \frac{1}{m}\right)\sigma^2(K)\right]$$

Equation (3) and equation (2) are equivalent for arbitrary $m$ only in the limit that $\sigma^2 \to 0$. The assumption that equation (3) could be exact in any dimension, at least for log-normally distributed values of $K$, is referred to as the Matheron conjecture (Matheron, 1963). It is indeed known (e.g., Rubin, 2003) to be correct for $m=1$. However, De Wit (1995) has shown that equation (3) is also equivalent to a truncated perturbation expansion in the case of general dimensionality. Note, however, that both equation (2) and equation (3) generate $K_{\text{eff}} = K_{GM}$ for $m=2$ (in two dimensions). Partly for this reason, the geometric mean $K$ value has received some attention. The geometric mean value of the hydraulic conductivity is also the median value of any log-symmetrical distribution, such as the log-normal form.

Because effective medium approximations are generated by equating a medium plus a typical heterogeneity with the medium itself, the effective conductivity appears both in an
input and an output and the resulting equations are always represented self-consistently (e.g., Kirkpatrick, 1973; Tinga et al., 1973). The disadvantage of effective-medium approximations is that they “all assume that the macroscopic system is homogeneous and generally fail to predict the properties of a multiphase medium close to the percolation threshold due to long-range correlations (Wikipedia).” In the present thesis I will be considering bimodal distributions with each mode described by a log-normal distribution. Since an effective medium approximation has been given (Rubin, 2003) for a similar problem, it is important to reproduce the result here,

\[ K_{\text{eff}} = \frac{1}{3} \left[ \frac{V_{\text{clay}}}{K_{\text{clay}} + 2K_{\text{eff}}} + \frac{V_{\text{sand}}}{K_{\text{sand}} + 2K_{\text{eff}}} \right] \]

Equation (4) was derived (Rubin, 2003) for the case that both modes of the distribution have zero variance, so that \( K_{\text{clay}} \) and \( K_{\text{sand}} \) refer to the hydraulic conductivities of clay and sand respectively. When I apply equation (4) for the case of non-zero variance of the individual modes of the distribution, the meanings of \( K_{\text{clay}} \) and \( K_{\text{sand}} \) must change to the geometric means of the distribution of clay and sand conductivity values. Use of equation (4) for the narrower distributions assumed in Rubin (2003) should normally produce a \( K_{\text{eff}} \) with accentuated sensitivity to changes in sand content near the onset of global connectivity (percolation) of the sand, but it was not possible to test this hypothesis. Note that the
effective conductivity of the medium, $K_{\text{eff}}$, appears on both sides permitting an iterative solution of equation (4).

In their conclusions Scheibe and Yabusaki (1998) advised against using effective $K$ values, whether calculated from equation (1) or otherwise, because effective parameters can be “ill-defined” due to “geometric patterns which give rise to preferential flow and transport pathways” and “multiple scales of nested heterogeneity.” Other authors (Knudby and Carrera, 2006) have concurred, emphasizing the underappreciated role of connectivity of highly conducting pathways. However, when an analytical formula is desired, power-law averaging as in equation (1) has frequently been given as a means to evaluate the effective hydraulic conductivity (e.g., Deutsch 1989; Desbarats, 1992). I can criticize power-law averaging schemes such as the Scheibe and Yabusaki (1998) treatment based on the observations of Bernabe and Bruderer (1998), which force thinking based on percolation theory. Bernabe and Bruderer (1998), among others, have used numerical simulations to show that, as in critical path analysis, the most important conductivity values of a distribution are somewhere between the minimum and maximum values, in contrast to the construction of Scheibe and Yabusaki (1998), which places them either at the minimum or the maximum, and has, furthermore, no representation of the connectivity of sites. Thus, two commonly used upscaling schemes, stochastic (Matheron 1967) and power-law averaging (e.g., Scheibe and Yabusaki, 1998) are limited either conceptually (power-law averaging), or practically (stochastic). Thus it makes sense to turn to percolation theoretical techniques (particularly as they also quantify connectivity).
Appropriate percolation theoretical procedures can be formulated under two widely different conditions; near, and far above the percolation threshold. These two general formulations can be labeled percolation path analysis (PPA) and critical path analysis (CPA) respectively. Percolation path analysis is our term for standard percolation scaling (Stauffer and Aharony, 1994). The second method will have a strong dependence on the distribution \( W(K) \) of the medium while the first is more closely related to the topology of the path. Both methods have been used accurately in the prediction of DC and low frequency AC electrical conductivity (Hunt, 2001b, McLachlan et al., 2007), where the electrical conductivity has many similarities with hydraulic conductivity, as well as in pore-scale calculations of the saturated (Katz and Thompson, 1985) and unsaturated hydraulic conductivity (Hunt, 2005).

The chief method developed here is a kind of hybrid treatment. This method is mathematically based on percolation theory, which was chosen because large variances in \( K \) can thereby be treated within a theoretical framework based on a quantitative theory of connectivity. But it was inspired also by the work of Scheibe and Yabusaki (1998) in their attempt to find a universally applicable algorithmic upscaling approach. In addition, a novel scaling method will be discussed. This treatment is also inspired by the work of Scheibe and Yabusaki (1998), but can be justified in terms of a result from fundamental physics (Halliday, 1993) relating conductance and conductivity.
The general purpose of the work here is to test upscaling methods on models of a medium, which are as realistic as possible. Thus some discussion of such models is required. The most realistic model appears to be that of Ritzi and Dominic (2005) based on field work of Bridge et al. (2000) Lunt and Bridge (2004) and Lunt et al. (2004). The field data were extracted by various means from an Arctic braid-belt sequence of the Sagavanirktok River. While future work will be based on this model, it was not available in time to be used here. Instead I used a model developed by Guin and Ritzi (2008); each of these models (Ritzi and Dominic, 2005; and Guin and Ritzi, 2008) was developed along the same general lines as the model of Scheibe and Freyberg (1995). That model was based on detailed sedimentological information from Basumalick (1966), Pryor (1973) and Jackson (1976). The most important advances in the model of Ritzi and Dominic (2005) are related to its size, which encompasses trillions, instead of merely millions, of nodes. The increase in size then allows an increase in the number of spatial scales that are explicitly represented. An additional improvement is the use of realistic statistics of $K$ distributions (Guin and Ritzi, 2008) rather than the idealizations of log-normal distributions, a change which can be incorporated into the upscaling techniques introduced here.

The hierarchical nature of all of these models is argued to be important for representing reality; as the scale of observation is increased, one finds different facies assemblages. Thus, macroform assemblages allow varying statistics of the occurrence of point bar sequences relative to overbank deposits, while a point bar sequence allows realistic shapes and statistical occurrence of mesoforms appropriate to a point bar (figure 1). However, a
relatively simple version of such a hierarchical model can be constructed using only two sediment types (e.g. mud and sand), whose shapes, orientations, and correlations are scale-dependent, and whose statistical occurrences (microform assemblages) are correlated within mesoforms as well as macroforms. If each sediment type, sand or mud, has its own distribution of hydraulic conductivity values, the distribution of $K$ values at the largest scales may be represented in terms of a bimodal distribution as in Figure 1f (Level IV).

Because I was unable to test the theoretical constructions on the full Sagavanirktok River model, I test the theory on two simple 3D cubic models, each with bimodal distributions of the hydraulic conductivity. The first model will have a correlated cluster distribution of $K$, and the second will have a random cluster distribution of $K$. For both models I will use log-normal distribution, thus ensuring positive hydraulic conductivity values and a somewhat realistic distribution of hydraulic conductivities. In each model, there will be three possible scenarios (table1), either the two modes of the distribution are far from each other (difference of more than 5 orders of magnitude of between the mean values), or they will be close to each other yet with no overlap (difference of more than 3 orders of magnitude between the mean values), or will have an overlap (difference of 2 orders of magnitude between the mean values). Figures 2 through 4 show the histogram distribution for each scenario. The range of distributions resembles different possible geologic distribution of material, for example, the first scenario could resemble coarse sand and clay/silt, while the third scenario could resemble coarse sand and fine sand.
Figure 1: a&b) Hierarchical sedimentary architecture within a point bar deposit. c-f) corresponding hierarchy of permeability modes (From Ritzi et al, 2004)
For each case I will test percolation path analysis, critical path analysis and novel scaling by comparing them to hydraulic conductivity values computed from the water budget from simulations of a finite-difference code by McDonald & Harbaugh (1988) that iterates the differences in head for each node of the model, until it reaches a pre-set convergence criterion. The finite-difference code is one of the most commonly used programs for simulating ground-water flow. In general, the finite-difference method consists of one equation of mass balance for each cell in a lattice. Fluid is moved between adjacent cells according to these equations with fluxes proportional to a potential difference. Figure 5 illustrates a cubic lattice both in percolation theory and in finite-difference representation. As defined in the equations of mass balance fluids can only move between cells with a face-to-face connection. Thus a cell can only have a hydraulic connection with the cells above, below, north, south, east and west of the cell. The simple cubic lattice in site percolation theory is also defined with face-to-face connections among adjacent, occupied sites making simple cubic percolation probabilities relevant (see section on percolation theory). The code was used to solve for head values with confined boundaries under steady state conditions. The water budget ($Q$) calculated by the simulation is used to calculate the effective hydraulic conductivity ($K_{eff}$) of the model according to Darcy’s Law:

$$Q = K_{eff} \cdot \frac{\partial h}{\partial x}$$
Table 1 - Distribution of Hydraulic Conductivity Values.

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<tr>
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<th>Lower Dist</th>
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<th>Upper Dist</th>
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<tr>
<td></td>
<td>Arithmetic Mean</td>
<td>Variance</td>
<td>Arithmetic Mean</td>
<td>Variance</td>
</tr>
<tr>
<td>Log-Normal Dist.</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Large difference</td>
<td>7.83E-03</td>
<td>2.14E-05</td>
<td>1.27E+03</td>
<td>5.68E+05</td>
</tr>
<tr>
<td>between the means</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Medium difference</td>
<td>1.16E+00</td>
<td>4.72E-01</td>
<td>1.27E+03</td>
<td>5.68E+05</td>
</tr>
<tr>
<td>between the means</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Small difference</td>
<td>1.16E+00</td>
<td>4.72E-01</td>
<td>1.72E+02</td>
<td>1.04E+04</td>
</tr>
<tr>
<td>between the means</td>
<td></td>
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Figure 2: Histogram showing the distribution of hydraulic conductivity values for log-normal distribution with over five orders of magnitude difference in the mean value.
Figure 3: Histogram showing the distribution of hydraulic conductivity values for log-normal distribution with over three orders of magnitude difference in the mean value.
Figure 4: Histogram showing the distribution of hydraulic conductivity values for log-normal distribution with two orders of magnitude difference in the mean value.
Figure 5: An illustration of a simple cubic lattice that could be considered for site percolation theory or as a 3-D finite difference grid. Inserts shows that both a Cartesian system and an integrated index system are useful when referring to aspects of the lattice (From Guin, 2005).
Equation 5

\[ K_{eff} = \frac{Q}{A} \times \frac{dl}{dh} \]

where \( A \) is the cross-sectional area and \( \frac{dl}{dh} \) is the mean head gradient over the entire model. The hydraulic conductivity values from the simulation, \( K_{eff} \), are used as a benchmark (not necessarily ground-truth) for comparison with the various upscaling techniques.

Outputs of all three different upscaling methods applied to models with differing correlation structure and parameter values will be compared with the \( K_{eff} \) from simulation. Using these comparisons together with physical arguments regarding the reliability of each method, it should be possible to ascertain under what conditions each method can produce accurate results.

Some preventive procedures have been made to the run time and reach convergence of the mass balance. Some of these procedures are; a well discretized aquifer, and using a confined aquifer which limits the non-linearity introduced by a variable saturation thickness; and a large convergence criteria used for the distributions having large and medium mean separation.
The intellectual merit of the thesis is in its attempt to address relatively realistic distributions of hydraulic conductivity values. Previous results (Hunt, 2001a; Shah and Yortsos, 1996; Bernabe and Balberg, 1998) have shown that it is relatively straightforward to apply CPA to wide single-mode $K$ distributions, while it has also been easy to apply PPA to bimodal distributions, for which the individual modes are narrow and widely separated (Stauffer and Aharony, 1994). The novel scaling approach mentioned will be developed through analogy to PPA meaning that it should be accurate under the same conditions as PPA. Our purpose here, however, is to address the more realistic scenario that the individual modes of the distribution are wide enough that there may be some overlap between the two individual modes. Thus I propose to investigate under what ranges of conditions which of these three general analytical procedures has the greater success.

Percolation methods may also be useful in “Hybrid” treatments that upscale $K$. Thus, while it has been hoped that percolation methods may prove useful for predicting $K$ at any scale in a medium with many scales of variability, it may not be a good choice to use at all scales. Then, however, CPA may still replace more cumbersome finite element methods at smaller scales, allowing employment of full computational power at larger scales. Such an analysis may be particularly useful if at the largest scales macrostructures are not treatable in any statistical theory, but employing computational methods at all scales would be
impossible with current and future computational abilities. The formulated hypotheses will
have considerable relevance regarding *practical* applications of percolation theory (with its
random input) to a wider range of geologic media than those explicitly addressed.
II. Theory:

Percolation theory is a relatively recent development, having been invented in 1943 (Flory, 1943), but with considerable refinement continuing into the 1990’s (Stauffer, 1979; Stauffer, 1985; Sahimi and Yortsos, 1990; Sahimi, 1993; Bunde and Havlin, 1996, etc.). Its use in upscaling the hydraulic conductivity has been summarized in some reviews of percolation scaling concepts in the early 1990’s (Berkowitz and Balberg, 1993; Sahimi, 1993). The other stated avenue of upscaling the conductivity via critical path analysis is not based on scaling theory of percolation, but is even more recent, having been invented in 1971 (Ambegaokar et al., 1971; Pollak, 1972), and undergoing refinement up to the present (Hunt, 2005). The thesis will first discuss basic concepts in percolation theory. Then the use of percolation theory in upscaling will be introduced. The two principle techniques, Percolation Path Analysis (PPA), and Critical Path Analysis (CPA) will be described and how they can be adapted to upscale the hydraulic conductivity in our models. After that, the novel scaling method of upscaling will be discussed.

A. Percolation Theory:

Percolation theory describes the connectivity of objects (elements) with some defined spatial association. Spatial correlations between elements are neglected in the simplest version of percolation theory, but may be accommodated in more realistic applications. Indeed including such spatial correlations is an important component of the work proposed
here. Percolation theory has both universal and non-universal components and its results are relevant to both structure and conduction. The most commonly used applications to conduction include the interpretation of (mostly universal) power laws in a percolation parameter (Berkowitz and Balberg, 1993), though this may not be the most productive application, and is not the primary focus of the research proposed here.

Percolation theory may be applied to several rather different types of geometries: site, bond, and continuum. The first case was meant to describe applications to, e.g., the conductivity of mixtures of metal and plastic balls, with contact only between two nearest neighbor metallic balls providing a conducting connection. The second case was applied to describe the conduction properties of random resistor networks, with the individual resistors representing either conducting with a probability “\(P\)” or insulating bonds with a probability “\(1-P\)” on a network. The final case of continuum percolation is ideally suited to composite materials and porous media, where, for example, the limiting conduction process is not confined to contacts between particles or bonds between points. In all of these systems the restriction to conducting versus non-conducting elements may also be relaxed so as to allow application to systems with wide ranges of local conductance values, as are much more likely to be found in nature. In such applications there are three interrelated aspects of percolation theory that are critical to understand: 1) the concept of the critical percolation probability, 2) the correlation length, and 3) cluster statistics of percolation theory. In a nutshell, the critical percolation probability defines when an infinitely large cluster of interconnected sites, bonds, or volumes, first appears, the correlation length defines the linear dimension of the largest
cluster of interconnected sites (bonds or volumes), while cluster statistics yield the probability that a cluster of interconnected sites (or bonds or individual volumes) of a given total volume can be found (Stauffer, 1979; 1985).

Note that the effects of spatial correlations are incorporated into the upscaling of the hydraulic conductivity only in their impact on the critical percolation probability, $P_c$, and this impact on $P_c$ in the present model was, fortunately for the present study, already investigated by Guin and Ritzi (2008). It was previously known that geologic correlations tend to reduce the critical percolation probability (Silliman, 1990; Ioannidis and Chatzis, 1993; Garboczi et al., 1995), increasing an effective $K$. Although the value of the correlation length does not enter into calculations of an ensemble mean effective $K$, knowledge of its behavior will help to evaluate the importance of statistical fluctuations in both calculations and simulations.

Consider the simple cubic lattice, with the lattice extending to infinity. If $P$ is close to zero, most occupied sites will be isolated (figure 6). As $P$ increases, more isolated sites will be connected until at $P = P_c$ a cluster of interconnected sites will reach across the lattice. This value of $P = P_c$ is called the critical probability, and is also known as the percolation threshold. Therefore, an infinite lattice has a sharply defined percolation threshold or critical point at which a phase transition (from unconnected to connected) takes place. For $P > P_c$ a spanning cluster of sites exists while for $P < P_c$ no spanning cluster exists. In finite systems,
Figure 6: Definition of occupied clusters in a square lattice; shaded squares are occupied. The clusters are groups of neighboring squares with face-to-face connections. Clusters are encircled except when the cluster consists of a single square (From Guin, 2005).
however, there is no single value of $P_c$ and percolation occurs over a range of values of $P$, depending on the realization of the random variables.

1. Percolation Path Analysis:

Under some circumstances the conductivity, electrical or hydraulic, of site and bond percolation systems can be represented very simply. Consider for simplicity a bond percolation problem on a square lattice or grid in two dimensions. Let some fraction, $P$, of the connected bonds be conducting (all with identical conductivities), while another fraction, $1-P$, is insulating. Let there be no correlations in the placement of the conducting bonds. On a square lattice the bond percolation probability is known to be 0.5 (Stauffer and Aharony, 1994). Under such conditions it is known that the electrical conductivity ($\sigma$) must obey the following scaling relationship (Normand and Herrman, 1990),

**Equation 6**

$$\sigma = \sigma_0 (P - P_c)^{\frac{1}{3}} = \sigma_0 (P - 0.5)^{\frac{1}{3}}$$

where the second equality is restricted to the square lattice in bond percolation. Here $\sigma_0$ is a pre-factor with units of electrical conductivity, but the result would be exactly analogous if the hydraulic conductivity, $K$, were substituted. Addition of correlations to the placement of
conducting bonds (or substitution of another grid, such as triangular form) may change $P_c$ to another numerical value, but there will be no other change in equation (6) (Stauffer, 1994). The same result is obtained for site percolation problems, except that $P_c$ values again will be different. In three dimensions the same functional form is again obtained, but now the exponent is different as well (Gingold and Lobb, 1990; Clerc et al. 2000),

**Equation 7**

$$K = K_0 (P - P_c)^2$$

Equation (7) was written for the hydraulic conductivity in order to emphasize that such an equation applies to either electrical or hydraulic conductivity. Equation (7) can be adapted to the case that the conductances of the conducting bonds are distributed over a range of values; then $K_0$ is the geometric mean of the upper distribution of hydraulic conductivity values. Equation (7) can only predict an effective $K$ for $P>P_c$ because for $P<P_c$, the conducting portions of the medium do not percolate and the conductivity is identically zero. Equation (7) is identical in form for all three-dimensional site or bond percolation problems, and does not depend on the correlation structure of the conducting bonds although the numerical value of $P_c$ will change. The consistency of the power (1.3 in two dimensions, 2 in three dimensions) leads to its characterization as “universal” (Stauffer, 1994).
Equation (6) and equation (7) must be modified in case the insulating bonds are replaced with bonds that conduct, even though minimally. Then, even if the highly conducting bond fraction fails to percolate the network will conduct with conductivity at least as large as the conductivity of a network with $P$ for the highly conducting portions equal to zero. Thus, the limiting value of the conductivity when $P \to P_c$ is modified by adding another term, whose value is most naively represented as a constant (Ewing and Hunt, 2006), the constant used is hypothesized to be the geometric mean of the lower distribution. The effective $K$ for $P < P_c$ will then be:

**Equation 8**

$$K = GM_{\text{Lower Distribution}}$$

In continuum percolation problems the power may not be universal however (Kogut and Straley, 1979; Balberg, 1987). Thus Berkowitz and Balberg (1993) characterized the application of percolation theory to upscaling the hydraulic conductivity of porous media as a process requiring three steps: 1) finding a variable which can stand for the percolation variable $P$, 2) finding the appropriate value of its threshold, and 3) finding the appropriate power in the scaling relationship. However, application of percolation theory to upscaling $K$ is considerably more complicated (Hunt, 2005). Step 1 may be taken over from Balberg and Berkowitz (1993), but the rest of the procedure is different, and cannot be simplified to an algorithm. This will be better understood after I have discussed CPA (next).
2.  **Critical Path Analysis**

Critical Path Analysis (CPA) was introduced in the condensed matter physics community in the early 1970’s to treat the electrical conductivity of disordered semiconductors far above the percolation threshold (Ambegaokar et al., 1971; Pollak, 1972). It was found that, especially when local electrical conductances varied over many orders of magnitude (Seager and Pike, 1974) (and similarly with the hydraulic conductance Bernabe and Bruderer, 1998), this method was best suited to calculating the effective conductivity of the medium. The reason was that the bulk of the charge transport occurred along highly conducting paths reminiscent of the “flow channeling” described by Moreno and Tsang (1994).

The critical path analysis can be described using the following thought experiment designed to describe upscaling of $K$ at the pore scale. Begin with a three-dimensional pore network. Remove all the pores from the network and then replace them, in their original locations, in decreasing order of conductance (decreasing pore radius). While placing them monitor the change in the conductance (electrical or hydraulic); as the first few pores are replaced the conductivity will be zero. Once a sufficient number of pores have been emplaced, the network will conduct because spanning will occur. The last pores that were emplaced are labeled “the critical pores”, and have conductivities $K_c$ (analogous to $P_c$). All the previous pores added before will have a higher conductance than the critical pore. Since the pores are connected in series the conductivity of the path will be governed by the
conductance of the last pores (smallest) added. Continue adding the remainder of the network, but now all these additional pores have smaller conductances. Since their configuration is in parallel with the critical pore, the smaller pores will not appreciably affect the upscaled value of $K$. An analogous procedure can be formulated for upscaling at geologic scales and is expected to be among the most accurate non-numerical solutions under a wide range of conditions. In particular, most of the flow occurs along paths through the medium, for which the smallest conductance value is as large as possible, making such paths logical candidates for the flow channels discussed by Moreno and Tsang (1994), a fact that was already pointed out in Shah and Yortsos (1996).

Fully developed CPA typically involves some type of optimization between the effects of conductivity distribution and the topology of percolation theory (Friedman and Pollak, 1981; Stauffer and Aharony, 1994)). In order to avoid the necessity of evaluating this competition in the three special cases enumerated above I have developed a new algorithmic procedure to obtain $K$ directly from $W(K)$. This algorithm procedure is consistent with the ideas of CPA and is, at the same time inspired by to the power-law averaging described by Scheibe and Yabusaki (1998). Our method has been tested to give the correct results for upscaled $K$ for simple power-law distributions $W(K)$ in the cases $P_c = 0$ and $P_c = 1$, corresponding to parallel and series combinations of the individual resistances respectively (of course, so does the Scheibe and Yabusaki (1998) treatment). This procedure effectively finds the total resistance along a path which includes, in series, all the resistances less than the critical resistance. The statistical frequency of occurrence of each of the possible resistance values is, in a relative
sense, the same as in bulk, but rescaled so as to give a normalized probability. Then the value is multiplied by the ratio of the arithmetic mean conductance to the largest conductance in the system, as in this equation,

\[
K_{\text{eff}} = \frac{\text{Arithmetic Mean of } K_{\text{min}} < K < K_{\text{max}}}{K_{\text{max}}} \times \text{Harmonic Mean of } K_{c} < K < K_{\text{min}}
\]

\[
= \frac{\int_{K_{\text{min}}}^{K_{\text{max}}} K W(K) dK}{\int_{K_{\text{min}}}^{K_{\text{max}}} W(K) dK} \left[ \frac{1}{\int_{K_{c}}^{K_{\text{max}}} K^{-1} W(K) dK} \right]^{-1}
\]

It will be seen that, while such a method works quite well in a monomodal distribution, it generates some difficulties with bimodal distributions. One purpose of this thesis is to understand better these discrepancies.

Both of the procedures discussed above have a unique way of representing an optimal path utilized by the dominant flow characterizing the effective hydraulic conductivity. Critical path analysis generates the path of lowest resistance which if the system is far from percolation, should be a more accurate procedure for the upscaling. On the other hand, percolation path analysis is based on the topology/tortuosity of flow paths rather than the statistics of the conductance values. The percolation path analysis is then the most accurate upscaling technique close to but above the percolation threshold. The research will study the
cross-over in relevance from critical path analysis to percolation path analysis in different yet semi-realistic geological media.

3. Novel Scaling Approach

A novel scaling approach is proposed here for calculation of the hydraulic conductivity; it was inspired by the line of thought of Scheibe and Yabusaki (1998) and the PPA. Scheibe and Yabusaki (1998) assume that the hydraulic conductivity of two or more distributions is a power-law function (equation 1) that must clearly fall between the harmonic mean of the composite distribution and its arithmetic mean, while in PPA the hydraulic conductivity is assumed to have a scaling function accurate near and above $P_c$. The novel scaling approach refers to both ideas. Thus, the effective hydraulic conductivity below $P_c$ is a function of the volume fraction of the upper distribution ($P_s$ is the same as $P$) (equation 10), and the geometric mean of the entire distribution, while above $P_c$ the effective hydraulic conductivity is dependent on both the volume fraction and a scaling factor.

Equation 10

$$P_s = \frac{V_{\text{Upper Distribution}}}{V_{\text{Upper Distribution}} + V_{\text{Lower Distribution}}}$$

The method proposed has the same format as the PPA, but the values of hydraulic conductivity for $P_s < P_c$ is a function of $P_s$ and the geometric mean,
In equation (11) $GM$ is the geometric mean of the entire data set, $P_c$ is the critical percolation probability, and $P_s$ is the volume fraction of the upper distribution (defined in equation (10)). For simplicity I will consider the upper distribution as sand; “$GM$ of sand” is therefore generally the geometric mean of the upper distribution. For $P_s = 0$ the effective hydraulic conductivity will be equal to the geometric mean of the lower distribution, and at $P_s = 1$ the effective hydraulic conductivity will be equal to geometric mean of the upper distribution. The second term in equation (11) for $P > P_c$ makes implicit use of an isolation of topological and distribution effects on $K$ by employing a product analogous to the fundamental physics equation, $\sigma = gl/A$ (Halliday, 1993) with $\sigma$ the conductivity, $g$ the conductance, $l$ the system length, and $A$ its cross-sectional area. In particular the geometric mean conductivity takes the place of the product of the conductance $g$ and the length $l$ while the probability factor (from topology of percolation theory) substitutes for the inverse of the area $A$. 

\[
\begin{align*}
K_{\text{eff}} &= GM \times (1 - P_s) & \text{if } P < P_c \\
K_{\text{eff}} &= GM \times (1 - P_s) + GM \text{ of sand} \times \left( \frac{P_s - P_c}{1 - P_c} \right)^2 & \text{if } P > P_c
\end{align*}
\]

Equation 11
III. The Model

A probabilistic model for subsurface flow was generated using a cubic grid. The grid had a 10m length while each individual cell length was 0.1m. The grid was composed of \((10^3)^3=10^6\) cells. The simulations from Guin and Ritzi (2008) using Carle (1999) code was used to generate a probabilistic arrangement of local conductances in accord with a bimodal \(K\) distribution. The model generates assigned fractional volumes \((P_s)\) with respect to the upper distribution (equation 10). The procedure to generate a correlated distribution is quoted from Guin (2005) in the following.

“The TSIM code by Carle (1999) is used here to generate realizations of sand and clay distributions. The TSIM code generates the realization through a two-step procedure: (A) sequential indicator simulation; (B) simulated quenching.

A. Sequential Indicator Simulation:

Sequential indicator simulation is fast, robust and conceptually easy to understand. It is the most widely used, non-Gaussian simulation technique (Deustch and Journel, 1998). It is based on cokriging estimation, in a nearest-neighbor sense, to estimate the local probability distribution while honoring global statistics and transition probability structures (Carle, 1999). The approach permits correlation between contiguous simulated values.”
In the indicator simulation approach, the number of indicator categories is defined by the indicator variable $I(i,j,k)$ (equation 12), where the indices $i, j, k$ denote cells in the $x, y,$ and $z$ coordinates.

**Equation 12**

\[ I_s(i, j, k) = \begin{cases} 1 & \text{if a sand cell} \\ 0 & \text{otherwise} \end{cases} \]

“A regular grid network of cells is then defined at which estimates will be made. Grid cells are chosen sequentially along a random path; the following four steps are performed at each ‘unsimulated’ grid cell location:

a. A search is conducted at each grid cell $(i, j, k)$ for nearby data locations.

b. A local conditional cumulative distribution function is estimated by transition probability based cokriging values conditioned to the already simulated data nearby. This is a step function defining the probability of each category occurring.

c. A random number between 0 and 1 is chosen.

d. The cell is assigned an integer indicator based on the interval in the cumulative distribution function into which the random number falls.

At each unsimulated grid cell, these four steps are repeated, with cokriging estimates conditioned to the sequentially updated version of simulation (Carle, 1996).

If multiple simulations are to be performed, the above algorithm is repeated, starting at a different initial grid location and visiting grid nodes in a different order each time.
B. Simulated Quenching:

The simulated quenching step improves the simulation in terms of matching simulated and modeled transition probabilities. The quenching step attempts to solve the optimizing problem of

**Equation 13**

\[
\min \{ O = \left[ t_{a\beta} (h_y)_{SIM} - t_{a\beta} (h_y)_{MOD} \right]^2 \}
\]

where “\(O\)” denotes an objective function, and ‘SIM’ and ‘MOD’ distinguish simulated (measured from simulation) and modeled (input) transition probabilities (Carle, 1999). This step is implemented by repeatedly cycling through each cell of the simulation and inquiring whether a change to another category will minimize [sic] \(O\); if so, the change is accepted. This iterative process continues until \(O\) is minimized (Carle, 1999).

The same code can be used to simulate random placement of sites within the lattice by using a correlation range much smaller than the size of a single cell, in essence creating no correlation.”

The geological correlation length \((l(\mu))\) for the correlated and uncorrelated model is calculated according to equation 14 and 15 respectively (Guin and Ritzi, 2008):
Equation 14
\[ \tilde{l}(u_y) = \frac{1}{(1 - P_s)} \delta y \]

Equation 15
\[ \tilde{l}(u_y) = \frac{10}{(1 - P_s)} \delta y \]

The combined correlation length \(L(\tilde{u}_y))\) is calculated according to the equation 16 (Table 2) (Hunt, 2005):

Equation 16
\[ L(\tilde{u}_y) = \tilde{l}(u_y) \times [\left( \frac{P_s - P_c}{1 - P_c} \right)^{0.88} ] \]

The cube of the combined correlation length is effectively a representative elementary volume (REV) (Berkowitz and Balberg, 1993; Hunt, 2001a). When the combined correlation length is much larger than the system size (Table 2), the hydraulic conductivity values show a strong dependence on realization (Berkowitz and Balberg, 1993; Hunt, 2001a, 2005), making \(K_{eff}\) uncertain. In isotropic systems finite-size corrections will tend to increase an
ensemble mean value of $K$ (Hunt, 2001a) relative to $K_{\text{eff}}$ in an infinite system. Such corrections have not been incorporated here. In any case I generated three simulations for each data set and took the ensemble mean of the simulations to reduce the uncertainty. However, the simulations differed only in the assignment of the conductivity values to each unit type (e.g., sand and clay) while the spatial structure of the simulation did not vary for different simulations with the same $P_c$. As a consequence the most important characteristics, i.e., whether or not the more conducting unit percolates in a given realization, are reproduced in successive simulations.
Table 2 – Correlation length at various $P_s$

<table>
<thead>
<tr>
<th>$P_s$</th>
<th>Correlated</th>
<th></th>
<th></th>
<th>Random</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Geologic correlation length</td>
<td>Combined correlation length</td>
<td></td>
<td>Mean Length of Upper distribution</td>
<td>Combined correlation length</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.2758</td>
<td>1.380834024</td>
<td>$\infty$</td>
<td><strong>0.3116</strong></td>
<td>0.14526438</td>
<td>$\infty$</td>
<td></td>
<td></td>
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<tr>
<td>0.276</td>
<td>1.38121547</td>
<td>1870.813675</td>
<td>0.312</td>
<td>0.14534884</td>
<td>102.305442</td>
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<td></td>
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<tr>
<td>0.28</td>
<td>1.388888889</td>
<td>129.0873324</td>
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<td>0.14705882</td>
<td>7.1027293</td>
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<tr>
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<td></td>
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<td>1.95063096</td>
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<td></td>
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<td>$\infty$</td>
<td>$\infty$</td>
<td>1</td>
<td>$\infty$</td>
<td>$\infty$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
IV. Methodology

The critical percolation probability for the given simulation was obtained from Guin and Ritzi (2008). For uncorrelated sedimentary deposits, \( P_c = 0.3116 \) (cubic, site percolation value, Stauffer and Aharony, 1994), but for the correlated case Guin and Ritzi (2008) obtained \( P_c = 0.2758 \). It is important that this value of \( P_c \) was obtained from a single sequence of simulations with different \( P_s \) values.

The simulated data for the correlated sediments were generated by:

1. Producing data sets with 1’s and 0’s for correlated distribution having different proportions of 0’s and 1’s. The proportions used are listed in table 2.

2. Assigning hydraulic conductivity values for 0’s and 1’s, having a log-normal distribution (table 1).

After the data were generated, the following operations were performed:

1. Calculation for each data set of the geometric mean, arithmetic mean and harmonic mean for each distribution. Then the data was sorted in a descending order according to the hydraulic conductivity values; and the harmonic mean of values falling between the maximum and the critical percolation probability, \( P_c = 27.58\% \) of data points was calculated. The value thereby calculated is referred to as “the critical path summation”.

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2. Calculation of the CPA for each run (equation 9) utilizing the product of the critical path summation \( (K_c) \) and the arithmetic mean of the entire data points and subsequent division by the highest value of \( K \). The \( K_c \) was calculated by sorting the \( K \) values in a descending order, then calculating the harmonic mean values falling above the \( K \) value representing \( P_c \) (for correlated it would be the 275800 node). The highest value of \( K \) used was the mean of the higher distribution plus four times the variance. The use of four times the variance will exceed more than 99.9% of the data points, and simultaneously have a uniform value for all the calculations.

3. Calculation of the PPA and Novel Scaling according to equations 7 and 8 respectively.

4. Implementation of the finite-difference code using the data points generated in step 2, to calculate an effective \( K \) for each run.

The same procedure was then utilized for another set of points with the condition that the \( K \) distributions could overlap, then the same procedure was done for the random distribution data sets, while using a percolation threshold of 0.3116 (Guin and Ritzi, 2008). The steps performed to gather the data are summarized in the flow chart below.
Assign K values for the 0’s and 1’s

K-effective (simulation)

Calculate the Geometric Mean
  - Novel Scaling
  - PPA

Calculate the Harmonic Mean
  - Calculate the Critical Path Summation

Calculate the Arithmetic Mean

Sort the K values in an descending order

Generate data set (1’s and 0’s) for a specified $P_x$
V. Results

Figures 7 to 10 illustrate the realizations, both random and correlated, for five values of $P_s$ (0.1, 0.25, 0.35, and 0.2758). As shown in the figures the correlated sediments occur in groups in contrast to the random sediments that exhibit a dot like distribution (except in 3-D near and above the percolation threshold).

Figure 11 compares the hydraulic conductivity values generated by the simulation for random and correlated sediments. The distribution in both random and correlated sediments has 3 orders of magnitude difference between the means. As expected the correlated model generates a larger effective hydraulic conductivity. Also the increase in the hydraulic conductivity of correlated sediments does not increase smoothly, in contrast to the smooth curve that the simulation generates in the random distribution. This indicates a potential uncertainty in the $K_{\text{eff}}$. Note that the region in which the curve appears to exhibit the relevance of fluctuations is $0.15<P_s<0.3$. The correlation length is on the order of the size of the system (Table 2) for $0.2<P_s<0.35$, in reasonably close correspondence with the simulation. Similar results are seen in all other simulations of $K_{\text{eff}}$ in correlated media.

Figures 12 to 17 illustrate for each model and each scenario, how the effective hydraulic conductivity values changes as the $P_s$ changes. As shown in the figures, for a correlated model the effective hydraulic conductivity falls between the geometric mean and the
Figure 7: Three-dimensional realization of a cubic lattice at $P_s = 0.10$ for both correlated (left) and random (right) systems (From Guin, 2005).
Figure 8: Three-dimensional realization of a cubic lattice at $P_s = 0.25$ for both correlated (left) and random (right) systems (From Guin, 2005).
Figure 9: Three-dimensional realization of a cubic lattice at $P_s = 0.35$ for both correlated (left) and random (right) systems (From Guin, 2005).
Figure 10: Three-dimensional correlated realization of a cubic lattice right at $P_s = P_c = 0.2758$ (From Guin, 2005).
Figure 11: Comparison of the hydraulic conductivity values of correlated medium (blue) and uncorrelated medium as a function of sand fraction $P_s$. In both scenarios the medium has a large peak variance.
Figure 12: Comparison of various mean $K$ values (geometric, arithmetic, harmonic) with simulation ($K_{\text{eff}}$) result (in purple) for an effective hydraulic conductivity as a function of sand fraction $P_s$. Sediment deposits are correlated (with correlation length above 1). Distribution of individual $K$ values covers over five orders of magnitude.
Figure 13: Comparison of various mean $K$ values (geometric, arithmetic, harmonic) with simulation ($K_{eff}$) result (in purple) for an effective hydraulic conductivity as a function of sand fraction $P_s$. Sediment deposits are correlated (with correlation length above 1). Distribution of individual $K$ values covers three orders of magnitude.
Figure 14: Comparison of various mean $K$ values (geometric, arithmetic, harmonic) with simulation ($K_{eff}$) result (in purple) for an effective hydraulic conductivity as a function of sand fraction $P_s$. Sediment deposits are correlated (with correlation length above 1). Distribution of individual $K$ values covers two orders of magnitude.
Figure 15: Comparison of various mean $K$ values (geometric, arithmetic, harmonic) with simulation ($K_{eff}$) result (in purple) for an effective hydraulic conductivity as a function of sand fraction $P_s$. Sediment deposits are effectively uncorrelated (correlation length smaller than grid size). Distribution of individual $K$ values covers over five orders of magnitude.
Figure 16: Comparison of various mean $K$ values (geometric, arithmetic, harmonic) with simulation ($K_{eff}$) result (in purple) for an effective hydraulic conductivity as a function of sand fraction $P_s$. Sediment deposits are effectively uncorrelated (correlation length smaller than grid size). Distribution of individual $K$ values covers three orders of magnitude.
Approximation for effective $K$-values for uncorrelated medium

Figure 17: Comparison of various mean $K$ values (geometric, arithmetic, harmonic) with simulation ($K_{eff}$) result (in purple) for an effective hydraulic conductivity as a function of sand fraction $P_s$. Sediment deposits are effectively uncorrelated (correlation length smaller than grid size). Distribution of individual $K$ values covers two orders of magnitude.
Figure 18: Comparison of results of techniques for upscaling hydraulic conductivity values with numerical simulation ($K_{eff}$), as a function of sand fraction $P_s$. Medium is composed of correlated sediments with large peak separation.
Figure 19: Comparison of results of techniques for upscaling hydraulic conductivity values with numerical simulation ($K_{eff}$), as a function of sand fraction $P_s$. Medium is composed of correlated sediments with medium peak separation.
Figure 20: Comparison of results of techniques for upscaling hydraulic conductivity values with numerical simulation ($K_{eff}$), as a function of sand fraction $P_s$. Medium is composed of correlated sediments with small peak separation.
Effective $K$-values for uncorrelated media from various techniques

Figure 21: Comparison of results of techniques for upscaling hydraulic conductivity values with numerical simulation ($K_{eff}$), as a function of sand fraction $P_s$. Medium is composed of effectively uncorrelated sediments with large peak separation.
Figure 22: Comparison of results of techniques for upscaling hydraulic conductivity values with numerical simulation ($K_{eff}$), as a function of sand fraction $P_s$. Medium is composed of effectively uncorrelated sediments with medium peak separation.
Figure 23: Comparison of results of techniques for upscaling hydraulic conductivity values with numerical simulation ($K_{eff}$), as a function of sand fraction $P_s$. Medium is composed of effectively uncorrelated sediments with small peak separation.
<table>
<thead>
<tr>
<th>Correlated</th>
<th>Large Mean Separation</th>
<th>All</th>
<th>Below Pc (0 – 0.27)</th>
<th>At Pc (0.275 – 0.28)</th>
<th>Above Pc (0.28 – 0.7)</th>
<th>Near P = 1 (0.7 – 0.1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>All</td>
<td>CPA</td>
<td>2.41</td>
<td>3.51</td>
<td>0.58</td>
<td>0.03</td>
<td>0.13</td>
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<th>Above Pc (0.28 – 0.7)</th>
<th>Near P = 1 (0.7 – 0.1)</th>
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Table 3 – RMSE results for various upscaling techniques for correlated sediments.
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<td>1.69</td>
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<td><strong>0.01</strong></td>
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<td><strong>0.02</strong></td>
<td>0.15</td>
<td>1.77</td>
<td>0.69</td>
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<td>Above Pc (0.32 – 0.7)</td>
<td>0.74</td>
<td>0.38</td>
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<tr>
<td>All</td>
<td>0.78</td>
<td>0.41</td>
<td><strong>0.05</strong></td>
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<td>Below Pc (0 – 0.31)</td>
<td>1.02</td>
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arithmetic mean. For the random distribution the effective hydraulic conductivity has an inflection point in the vicinity of \( P_c \), while at \( P_c \) the effective hydraulic conductivity is approximately equal to the geometric mean. When \( P_s = 0 \) and \( P_s = 1 \), the effective hydraulic conductivity will be approximately equal to the geometric mean values of the individual distributions of the lower and upper distributions respectively.

Figures 18 to 23 compares the CPA, PPA, the novel scaling method, and results from effective medium theory (EM - equation 4) used for the upscaling of hydraulic conductivities against the simulated effective hydraulic conductivities.

Note that in power-law averaging all the \( \mu > 0 \) (\( \mu < 0 \)) will produce a concave downward (upward) curve. Thus power law averaging cannot produce the observed sigmoidal shape which is a consequence of a cross-over from upward to downward curvature for \( P_s \approx P_c \). This failure to reproduce even the general structure of \( K_{\text{eff}} \) as a function of \( P_s \) led to its omission in the Figures. A conceptual model due to Gorelick and (), in which the effective \( K \) crosses over from the harmonic mean at low \( P_s \) to the arithmetic mean at high \( P_s \) captures the general structure, but does not recognize the role of percolation. If the percolation threshold were identified as the cross-over sand content, such a prediction might prove useful.

Table 3 (4) are the log percent root mean squared error (RMSE) calculation for the various techniques used for the upscaling of correlated (random) systems. I chose to use the
log values of the results to better represent smaller values. The RMSE was calculated according to the following equation:

\[
RMSE = \sqrt{\frac{\sum [\log(K_{\text{eff}}) - \log(K')]^2}{n}}
\]

where \( K' \) is the hydraulic conductivity of the technique used (CPA, PPA, Novel scaling, Arithmetic Mean...), \( n \) is the number of data points used. The RMS was calculated for the entire data points and for certain sections (below \( P_c \), at \( P_c \), above \( P_c \), and near \( P_s = 1 \)). The results in bold represent the best results calculated for a certain section.

Comparing the results from the correlated data, the CPA was able to predict the hydraulic conductivity in correlated simulations, but only in the region above the percolation threshold (0.25 till 0.6) for the overlapping, and (0.25 till 1) for the non-overlapping. For values lower than \( P_c \), various techniques resulted in better estimation for hydraulic conductivity, but none of the estimations is very good.

Comparing the results for the random data sets, the novel scaling method was able to predict to certain accuracy the simulated results for values near and above \( P_c \), while below \( P_c \) the novel scaling over estimated the hydraulic conductivity, this is more obvious for large mean difference. The CPA resulted in larger value above the percolation threshold, and underestimated the effective hydraulic conductivity below the percolation threshold.
The effective hydraulic conductivity values for both the random and the correlated simulations were not proportional to any mean values. The effective hydraulic conductivity was clearly closer to the geometric mean than to the arithmetic or harmonic mean for the entire simulations, although using the geometric mean of the entire distribution will never capture the rapid changes in effective $K$ when $P_s \approx P_c$. 
VI. Discussion

Some general statements regarding the expected dependence of the effective $K$ on $P_s$ will help to organize the following discussion. For $P_s = 0$, the effective $K$ is generated entirely within the lower mode of the distribution of $K$ values. For three-dimensional flow this value is greater than the median value, which for a log-normal distribution is the geometric mean. So, for $P_s = 0 K > GM$ (clay). For increasing $P_s$, $K$ increases, since the critical $K$ increases, but its increase is relatively slow until $P_s \approx P_c$, since in this range the critical $K$ remains in the lower mode of the distribution. For further increase in $P_s$, the critical $K$ jumps to the higher mode of the distribution, producing a much more rapid increase in $K$. This slope of $K$ vs. $P_s$ will of course increase when the separation of the modes of the distribution increases. For further increase in $P_s$, $K$ continues at first to increase rapidly for topological reasons – the connectivity of the paths through the higher conducting regions increases dramatically. Finally, when $P_s \gg P_c$, only a modest increase in $K$ with increasing $P_s$ is expected, since this reflects only an increase of the critical $K$ within the upper mode of the distribution. In all of these cases, the chief effect of correlations is to reduce $P_c$. Predictions of the simulations correspond more nearly to this scenario in the correlated cases than in the random cases.

The work presented here shows that the use of CPA for all correlated data sets resulted in accurate predictions near the percolation threshold and above the percolation threshold. While it had been hoped that it would also be accurate below the threshold, I found this not
to be the case. I attributed this failure to the division by a normalization factor, $K_{\text{max}}$, which was obtained from the upper mode of the distribution, and is thus too large a value for $P_s < P_c$. Conceptually I expect that in the range $P_s << P_c$, such a maximum $K$ value should correspond to the largest $K$ value in the lower mode of the distribution; in order to develop a useful prediction, a smooth interpolation between the individual $K_{\text{max}}$ values would be required. But I did not develop a physical argument to choose any particular such interpolation. The CPA was able to predict accurate results for both the overlapping and non-overlapping distributions.

For $P_s >> P_c$ and for long-range geologic correlations, percolation methods will tend to overestimate the tortuosity of the more highly conductive regions in a finite system. In such a case a single rather regularly shaped region of sand will span the system. The novel scaling approach will result in more accurate approximation under such conditions.

The version of CPA configured in this research does not have an accurate estimation of the hydraulic conductivity values below $P_c$, since it was developed for $P$ larger than $P_c$. But the CPA is supposed to have more accurate results, than the $K_{\text{eff}}$ from simulation for $P_s$ near $P_c$, because of uncertainty due to finite effects, where the $K_{\text{eff}}$ will vary from one simulation to another.
The model has another limitation, the effects of probability distribution of the clusters. The model will randomly assign the location of clusters, thus resulting in a different effective hydraulic conductivity value for the same $P_s$. This problem is especially noticeable for $P_s \approx P_c$. To avoid this limitation, multiple simulations should be conducted for the same $P_s$ and an ensemble mean developed. While multiple simulations will tend to improve the quality of $K_{eff}$ predictions near the percolation threshold, they may not remove all problems.

The PPA in all scenarios underestimated the hydraulic conductivity. The reason for such an underestimation is that the PPA only describes the topology of the path rather than considering the variability in the magnitudes of the $K$ values on the path. Nevertheless, under the conditions that the overlap in the distributions disappears and the widths of the individual distributions become negligibly small, PPA must generate the most accurate prediction (Stauffer and Aharony, 1994). I did not investigate this limit as it appeared to us to be less relevant to our attempts to describe the medium in a semi-realistic way. As a specific example PPA will be more accurate if I consider the lower distribution as a non-transmissive layer, where the water will not be able to move across the model if there is no spanning. Nevertheless, even here the accuracy of PPA will diminish as the width of the upper distribution increases.

The averaging method was an edited version of PPA to suit the needs of geology. It has the same format as the PPA, but I constrained the results to yield the geometric values of $K$ in
the limits $P_s \to 0$ and $P_s \to 1$, respectively. This method was able to estimate the effective hydraulic conductivity for the random model in all scenarios except for $P_s < P_c$ with a large mean difference.
VII. Conclusion

- For a correlated distribution, our critical path analysis (CPA) generates $K$ values in agreement with $K_{eff}$ from simulation for $P_s > P_c$. For $P_s < P_c$ CPA appears to underestimate the effective $K$ for reasons of a poor choice of normalization. In an uncorrelated medium CPA also generates predictions at variance from the simulations in the vicinity of $P_c$, where the effective $K$ generated by CPA exceeds that from the simulations.

- For an uncorrelated distribution for the entire range of $P_s$, the novel scaling approach more nearly coincides with the simulation than did CPA except for large differences in the mean where the novel scaling was not accurate. Since the novel scaling approach is based on PPA (which generates results based primarily on topology), then if the simulation is considered to be “ground truth”, the topological connections of the more permeable sediments have a greater influence than the details of the distribution of $K$ values. However, this topology near critical percolation is so complex (fractal in infinite spatial scales) that one might be skeptical of the ability of the simulation to fully represent it with the number of runs done. Thus I am yet unable to offer a clear judgment.

- Under the current conditions CPA (highly correlated, $P_s \geq P_c$) was able to predict the effective hydraulic conductivity in agreement with the simulation, this ability was not
affected by the width of the distributions, while the novel scaling was affected by the wide separation for values of $P_s < P_c$

- For $P_s >> P_c$ and for correlated systems the simplified topology of the sand units have a large impact on the effective hydraulic conductivity. Thus, under such conditions, the use of PPA or novel scaling approach will tend to generate a better estimation in both correlated and uncorrelated media.

- For $P_s \approx P_c$ the large value of the combined correlation length means that the system can never be treated as an REV (table 2). This introduces uncertainty into all calculation schemes.

- In most (of the six) cases one of the methods based on percolation theory performed best overall, but in two cases the effective-medium approximation (EMA) of Rubin (2003) generated the best over-all predictions. This was due mostly to a large failure in the percolation-based methods in some region of the curve and the EMA was unable to approximate the simulations closely in any region.
References


Gorelick


Appendix