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Multiple-point statistical prediction on fracture networks at Yucca Mountain

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Abstract In many underground nuclear waste repository systems, such as at Yucca Mountain, water flow rate and amount of water seepage into the waste emplacement drifts are mainly determined by hydrological properties of fracture network in the surrounding rock mass. Natural fracture network system is not easy to describe, especially with respect to its connectivity which is critically important for simulating the water flow field. In this paper, we introduced a new method for fracture network description and prediction, termed multi-point-statistics (MPS). The process of the MPS method is to record multiple-point statistics concerning the connectivity patterns of a fracture network from a known fracture map, and to reproduce multiple-scale training fracture patterns in a stochastic manner, implicitly and directly. It is applied to fracture data to study flow field behavior at the Yucca Mountain waste repository system. First, the MPS method is used to create a fracture network with an original fracture training image from Yucca Mountain dataset. After we adopt a harmonic and arithmetic average method to upscale the permeability to a coarse grid, THM simulation is carried out to study near-field water flow in the surrounding waste emplacement drifts. Our study shows that connectivity or patterns of fracture networks can be grasped and reconstructed by MPS methods. In theory, it will lead to better prediction of fracture system characteristics and flow behavior. Meanwhile, we can obtain variance from flow field, which gives us a way to quantify model uncertainty even in complicated coupled THM simulations. It indicates that MPS can potentially characterize and reconstruct natural fracture networks in a fractured rock mass with advantages of quantifying connectivity of fracture system and its simulation uncertainty simultaneously.

Keywords: multiple-point-statistics, fracture network, seepage, nuclear waste repository, Yucca Mountain

Introduction

Water flow rate and amount of water seepage into waste emplacement drifts is crucial for the performance of any underground nuclear waste repository, since this controls the mobilization rate of radionuclide and corrosion rates of waste packages. In many cases of underground nuclear waste repository, such as Yucca Mountain project, it is mainly determined by hydrological properties of fracture network in surrounding rock mass. Fracture-induced heterogeneity of water flow is the most important factor in determining whether and where seepage will occur for the variable saturation conditions at Yucca Mountain (Birkholzer et al. 1999). The spatial pattern of seepage into underground opening is a function of degree of permeability heterogeneity. This paper presents preliminary results of multi-point-statistical (MPS) prediction on fracture system and relevant flow behavior at Yucca Mountain, carried out under the framework of DECOVALEX-THMC project (Barr and Birkholzer 2005).

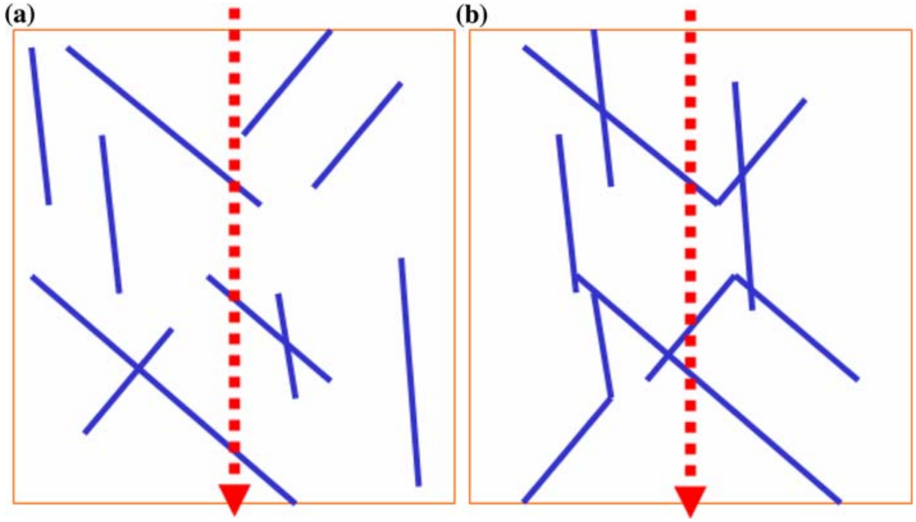


Fig. 1 Schematic of connectivity of fracture network (*Red dash* represents water flow through fractured rock mass, *blue lines* represent fractures)

Natural fracture network system is hard to describe fully, especially with respect to its connectivity which is critically important for simulating the water flow field. The characters of fracture system are not purely random though they are not regular. Therefore purely random-based prediction methods cannot fully characterize natural fracture system. Mathematical morphology provides a mean of fully characterizing a fracture network (Serra 1982). In general, there are three main kinds of survey: borehole survey, scanline survey, and areal survey. Areal survey can make it possible to retain more information than line-style survey though the traces always extend beyond 'survey rectangle' (Chilès and Marsily 1993). This type of survey is recommended for drift, tunnel walls, or outcrops. It is the exact equivalence of the spatial law for random functions. When probability distributions of trace length, density, fracture size, and orientation are determined basing on field survey of fracture system, one can reconstruct fracture network via stochastic simulation, such as conventional Monte Carlo sampling on known probability distributions. However, fracture information from filed survey is not fully utilized. As shown in Fig. 1, vertical water flows through two similar areas will be different even if two fracture network systems have same probability distribution of fracture density, orientation, and trace length. In other words, pattern of connected fractures or connectivity of fracture network is a very important character for water flow simulation in fractured rock, especially in sparsely fractured one. It indicates that some key information is lost in traditional characterization of fracture network, which controls the water flow. Discrete fracture network (DFN) model is validated not for its internal consistency, but for its usefulness in predicting fracture geometry and flow behavior in the rock mass. Large-scale observations in drifts and tunnels have also shown the clear effects of channeling flow, which refers to the phenomenon that liquid flow through a geologic system with its heterogeneous structure is focused along a few preferred pathways (Tsang and Neretnieks 1998; Tsang and Doughty 2003). It may reflect the nature of fracture intersection under special pattern of fracture network. Furthermore, these characteristic parameters of fracture network may vary locally, and then yield strong heterogeneity. Traditionally, each geometric parameter set characterizing the fracture networks (spacing, orientation, trace length) is described by a probability distribution law which type (e.g. uniform, Gaussian) is assumed to be constant over the volume of interest(Macè et al. 2004). The random parameter set is usually assumed to be stationary, even when considering the parameters of aperture distribution (Kim et al. 2004). Conventional method could only provide global stationary prediction of fracture network. It is necessary to develop a new method to take fracture network-specific heterogeneity into account, in spite of the great progress made during the past decades in characterizing and describing water flow in fracture rock mass. In this paper, a state-of-art geostatistical method for curvilinear geometries description in oil reservoirs simulation is introduced, instead of conventional geometric parameter set characterization and Monte Carlo sampling method, to describe fracture network in fractured rock mass.

In the following, we will first present MPS approach, and its application to fracture data from field observation to study flow field behavior at Yucca Mountain will be presented.

Multiple-point-statistical method

Geostatistics is a set of powerful methods for maps and mapmaking in the petroleum industry and mining. A map is a numerical model of an attribute's (e.g., porosity, permeability, thickness, structure) spatial distribution. Attribute mapping with high degree of confidence helps to make better flow prediction about the reservoir or reserve estimation of mine. Traditional geostatistics, including kriging, and more generally all regression-type maps are locally accurate in the minimum error variance sense, but because of smoothing, provide inaccurate representations of the spatial variability of the actual phenomena with various artifacts. It is the limitation of conventional simulation approaches based on two-point statistics (Deutsch and Journel 1998; Journel 1997; Srivastava 1995). Therefore, the use of smoothed maps is particularly inappropriate in cases where continuity/connectivity of extremes is important such as in the modeling of fluid flow in porous media (Schafmeister and Marsily 1993; Caers 2000). Curvilinear geometries cannot be modeled using only conventional 2-point geostatistics such as a variogram. Reproduction of such random geometric needs parameterization of specific shapes or the consideration of the joint categorical variability at three or more points at a time (Zhang et al. 2006). Therefore, specific geometries are poorly reproduced by conventional pixel-based algorithms, such as indicator or Gaussian truncated simulation techniques.

A new field, termed Multiple-Point Geostatistics or MPS, is rapidly rising. It does not rely on variogram models. Instead, it allows capturing inner structure from so-called 'training images', which are essentially a database of geological patterns. Multiple-point statistics borrows multiple-point patterns from the training image, and then anchors them to reconstructed simulation results (Caers 2000; Strebelle 2002; Zhang et al. 2006). Such method would account for correlations between three or more locations at a time. Hence, in theory, it would be able to reproduce the connectivity of many locations and thus reproduce complex, curvilinear geological structures. In current practice of curvilinear geometrical simulation, such as sinuous channels in a fluvial reservoir or incised valleys over topography, training images can be almost generated using unconditional object-based (Holden et al. 1998; Viseur 1999) or process-based (Wen et al. 1998) simulations.

Our approach on fracture prediction relies on a concept where fracture network is regarded as connected curvilinear geological structures. Geological structures, such as sand body in special shape and meandering channels in fluvial reservoir, may be products of multiphase tectonics and sedimentation in geologic history. Similarly, fracture system is caused by the initial stage of formation of rock mass and the successive tectonic motion processes. Therefore, there are intrinsic patterns in them which can be characterized in local survey area and reconstructed to a reasonably larger area via MPS means. The process of fracture description can be briefly summarized as following:

Grid-based discretization of fracture network as training image

Figure 2 shows how binary (fracture/matrix) grid is defined to describe fractured rock mass. Then vector fractures are transferred into grids with permeability defined as k_f (fracture-embedded grid) and k_m (matrix grid). The indicator notation is used for ti(u):

$$\mathrm{ti(u)} = \begin{cases} 1 & \text{if at u ti contains fracture} \\ 0 & \text{if at u ti contains matrix} \end{cases} \tag{1}$$

$\mathrm{ti_T(u)}$ is value of the training image ti where $u \in G_{ti}$, G_{ti} is the regular Cartesian grid discretizing the training image. It indicates a specific multiple-point vector of ti(u) value within a template T centered at grid node u.

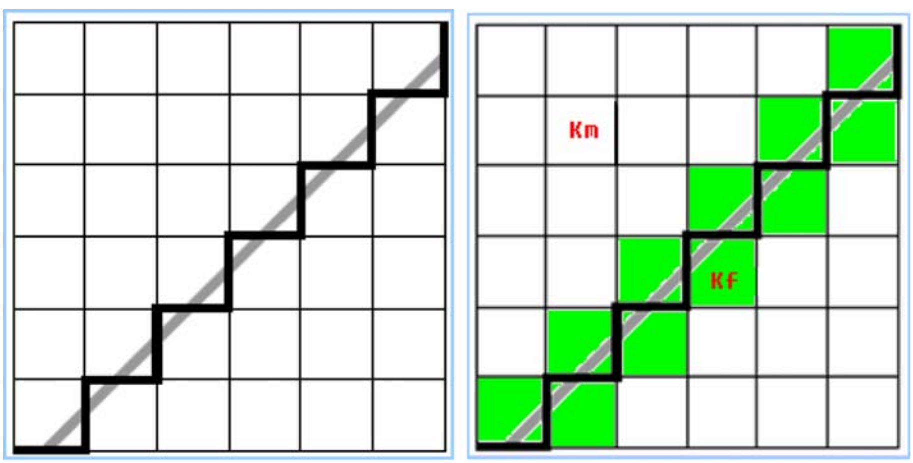


Fig. 2 Schematic of grid-based discretization of fracture network (binary-value (fracture/matrix) permeability representation of fracture (*grey line*))

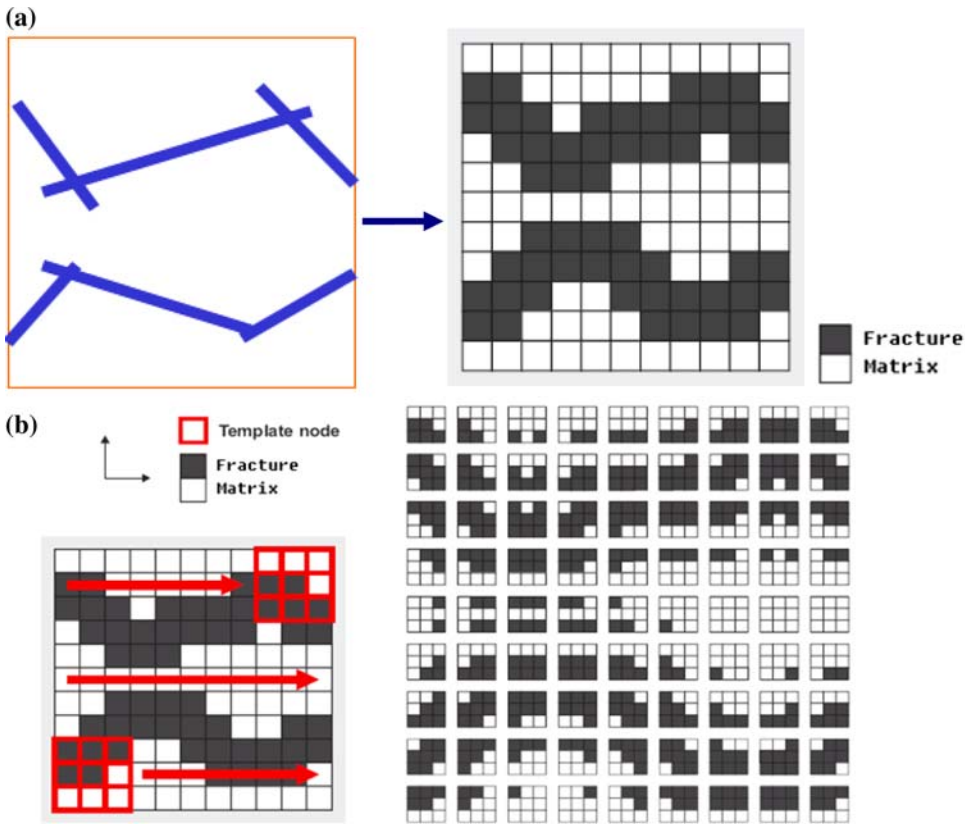


Fig. 3 Schematic of training image and pattern database in multiple-point statistics. (**a**) binary-value (fracture/matrix) grid representation of fracture network (*blue lines*); (**b**) scan on training image with specific template (multi-grid in *red*) to create pattern database)

Scanning of the training image to extract its constituent fracture patterns

The training image ti is scanned using template T (3 × 3 nodes in this study, shown in Fig. 3b) and storing the corresponding multiple-point $ti_T(u)$ vectors in a database. Each such $ti_T(u)$ vector is called a "pattern" of the training image and the database is called the "pattern database" which is denoted by pat_db_T. Once the patterns are stored in the pattern database pat_db_T, they are considered to be location independent, i.e. the database does not store the location $u \in G_{ti}$ of a pattern; only the content of the pattern is stored (Arpat 2005).

Sequential simulation with patterns

Once the pattern database pat_db_T is constructed, the algorithm proceeds with the simulation of these patterns on a realization re. Sequential simulation methods were developed, following the generic flowchart:

(1) Define a random path visiting all uninformed nodes.
(2) For each node u_α, draw the simulated value sampled from conditional distribution Function.
(3) Continue until all nodes on simulation grid have been simulated

A realization of grid-based fracture network is then reconstructed containing pattern information extracted from 'training image' of known fracture network maps.

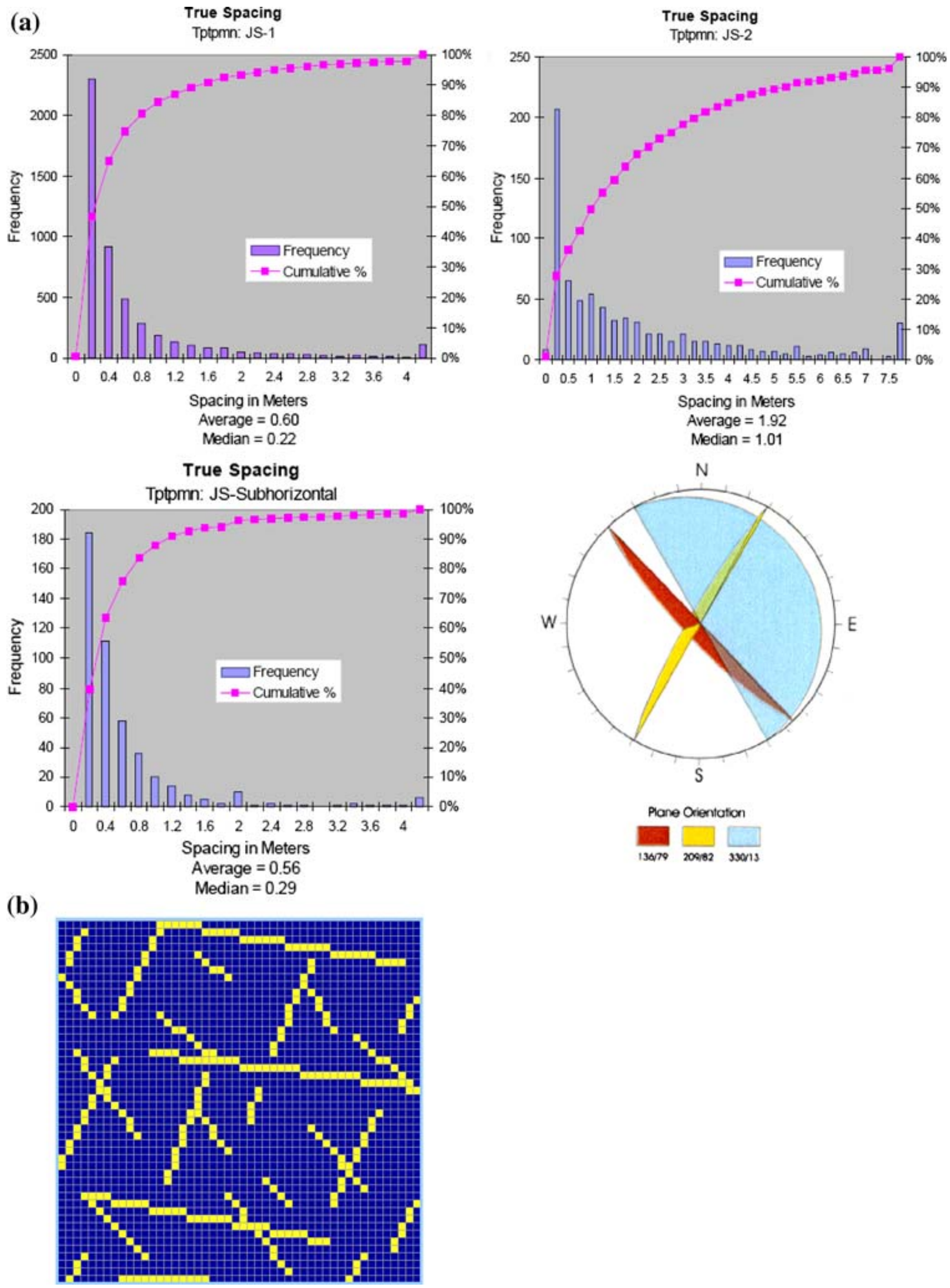
Reconstruction of fracture network at Yucca Mountain

Based on MPS method described earlier, we created grid-based discrete fracture network as training image. Input data for the training image creation are statistical distributions of geologically observed fracture spacing, and orientation trace lengths taken from Yucca Mountain datasets assembled by Hardin and Westermann (2000), shown in Fig. 4.

2D fractures system prediction

When the fracture 'training image' is ready, fracture patterns will be then extracted into a database by scanning of the training image. The goal of pattern recognition on fracture network is to classify observed fracture patterns into groups or classes. After pattern database pat_db_T is constructed, many realizations of fracture network are reconstructed by sequentially sampling on these patterns (described above). Spatial binary-value grids represent

Fig. 4 Fracture observations and artificial training image (in (**a**), fracture measurement data from Hardin and Westermann (2000)



rock blocks containing fracture and rock matrix. As shown in Fig. 6, realizations of grid-based fracture networks are simulated over the near field area around Yucca Mountain waste repository drift (80 m × 80 m). More fine grids (0.5 m × 0.5 m) are used in 10 m × 10 m area near drift. We can find that these realizations of fracture networks seem to have similar pattern for the human eye while they are obviously not in the same distribution of fracture. The recognition and reconstruction of fracture pattern or connectivity are realized statistically by MPS method, while they do not exist definitely in conventional means for fracture prediction.

Upscaling of permeability

Once a fracture network has been reconstructed, the equivalent permeability of the fracture network can be assessed. In order to do more efficient numerical simulation, large-scale continuum analyses using hydraulic equivalent properties should be adopted (Baghbanan and Jing 2007). In crystalline rocks with nearly negligible permeability of the rock matrix, the fracture system dominates the flow and permeability of the rock masses. Rock mass around Yucca Mountain repository drift can be described as a well-connected fracture network behaving

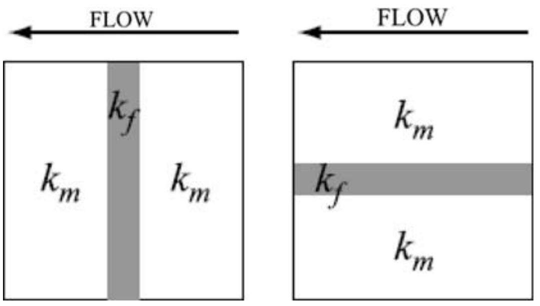


Fig. 5 Schematic of block permeability up-scaling (left for harmonic average, right for arithmetic average of permeability. k_f is permeability in fracture and k_m is permeability in matrix.)

similarly to a continuous and heterogeneous medium with considerable variation in permeability (Birkholzer and Tsang 1997). Determination of the equivalent hydraulic properties is very important for understanding the hydraulic behavior of fractured rock masses. In this study, we use a spatial average model (Pickup et al. 1995; Odling et al. 2004) to evaluate the permeability distribution of the fractured crystalline rocks. For flow along a grid element parallel to a fracture, the arithmetic average of permeability is used, and for flow along a grid element perpendicular to a fracture the harmonic average is used, as shown in Fig. 5. The appropriate permeability of blocks representing fracture can then be simply calculated using the formulae for adding permeability in series (2) and parallel (3).

$$\bar{k} = 1/\left[\frac{\sum_{i=1}^{N} t_i/k_i}{\sum_{i=1}^{N} t_i}\right] \tag{2}$$

$$\bar{k} = \left[\frac{\sum_{i=1}^{N} t_i \cdot k_i}{\sum_{i=1}^{N} t_i}\right] \tag{3}$$

where t_i is the thickness of each of the N layers and k_i is the corresponding permeability.

We adopt this harmonic and arithmetic average method with a line-by-line scan to upscale the permeability (k_f and k_m are set to values of fracture and matrix continuum, see Table 1) to a coarse grid (5 m × 5 m). Figure 7 shows realizations of whole area permeability after up-scaling and Yucca Mountain case simulation conditions. MPS simulations are carried out under conditions that average permeability is set to mean value of field measured permeability 7×10^{-17} [m^2] and permeability at top of drift surface is conditioned to measured value. Figure 8 shows comparison between MPS simulated and survey of permeability along the circumferential repository drift surface. It can be seen that there is good linear similarity between them and the correlation coefficient is about 0.86 when compared to pre-excavation permeability, which indicates that MPS simulation can grasp and recreate some natural patterns of fracture network near the repository. In fact, knowledge of spatial distribution of permeability is more important than its statistical distribution because the former

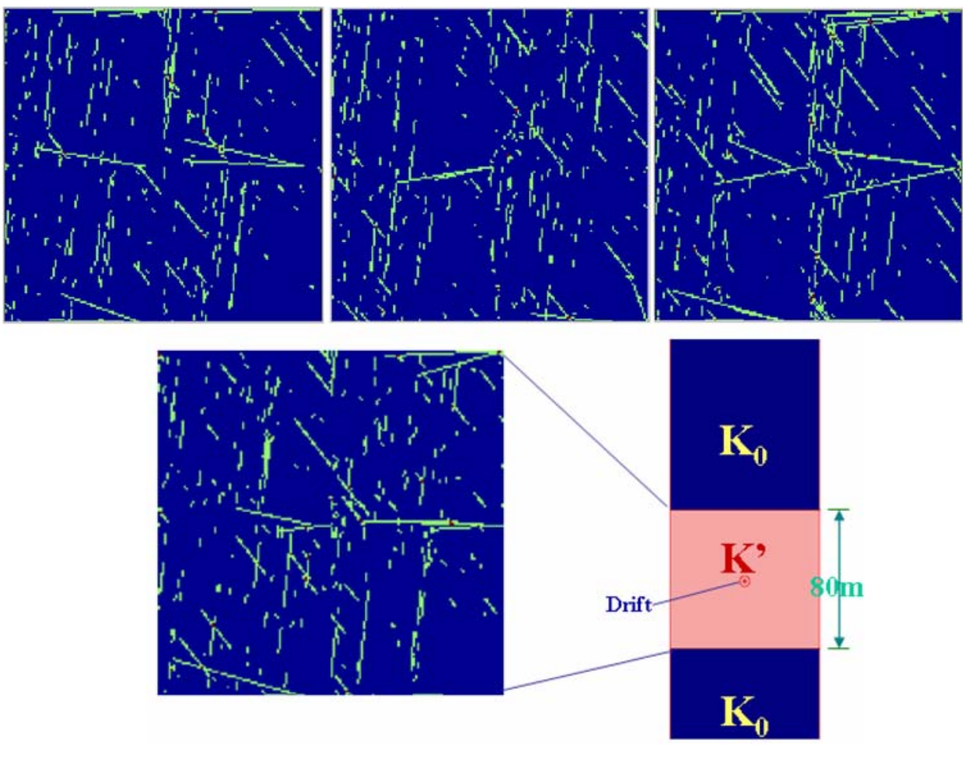


Fig. 6 Realizations of fracture network in 2.5 m × 2.5 m grid by MPS reconstruction (0.5 m × 0.5 m fine grids in 10 m × 10 m area near waste repository drift; red square in middle part represents simulation area near waste repository drift with variable permeability K'; K_0 is average permeability of rock mass)

Table 1 Properties of the rock mass in a dual continuum model used in Yucca Mountain case simulation

Type	Property	Value
Hydraulic properties of the fractured continuum	Permeability (m^2)	3.3×10^{-13}
	Porosity (−)	0.0083
	van Genuchten's air-entry pressure (kPa)	9.615
	van Genuchten's exponent, m(−)	0.633
	Residual saturation (−)	0.01
Hydraulic properties of the matrix continuum	Permeability (m^2)	1.77×10^{-19}
	Initial porosity (−)	0.13
	van Genuchten's air-entry pressure (kPa)	118.3
	van Genuchten's exponent m(−)	0.317
	Residual saturation (−)	0.19

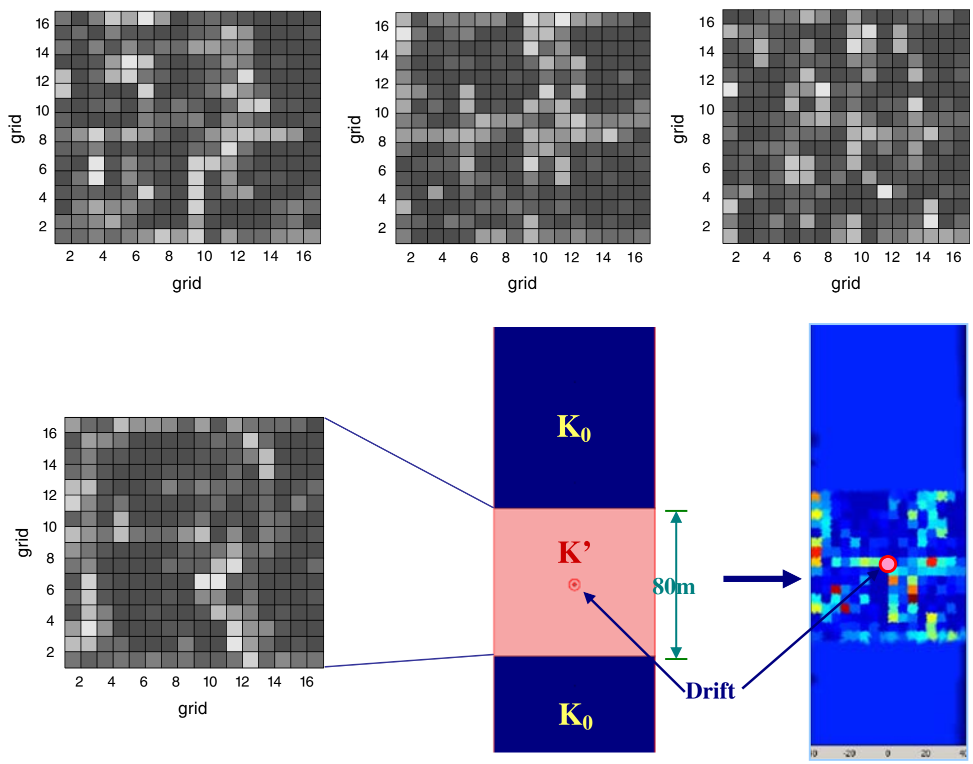


Fig. 7 Realizations of up-scaled permeability distribution in near field of repository drift (*red square* in middle part represents simulation area near waste repository drift with variable permeability K'; K_0 is average permeability of rock mass)

dominates heterogeneity and one can simulate more real water flow with it.

Analyses of fracture-distribution-induced seepage into drift

Flow field is solved by Fluid-Rock Transport simulator, coupled THM processes (FRT-THM) code being developed by the CAS team under DECOVALEX project. It is based on MATLAB and C language codes, in which FEMLAB^{TM} is used as partial differential equation solver (Liu et al. 2006). Basic parameters used in Yucca Mountain case simulation are listed in Tables 1 and 2, and numerical grids and boundary conditions are shown in Fig. 9. The top boundary, representing the ground surface was free to move, with a fixed water influx (6 mm/year), whereas the bottom boundary, representing water table had a vertical zero-displacement restriction for displacement, with a fixed pressure. The lateral boundaries (vertical sides of the model) are no-flux boundary for fluid and heat, with a zero-displacement restriction for the displacement normal to the boundary surfaces. The spatial permeability distribution for one realization is shown in Fig. 7, in which the mean value of permeability is set to 7×10^{-17} [m^2] for the purpose of comparison with uniform permeability.

As a result, water saturation distribution simulated with N fracture realizations are shown in Fig. 10. We can find obviously different flow fields from the same statistical

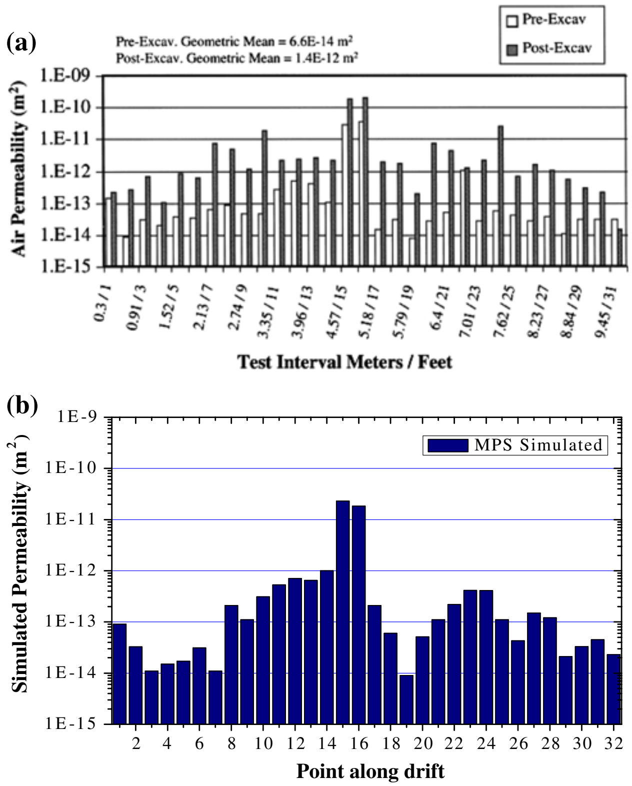


Fig. 8 Permeability along circumferential waste repository drift surface. (**a**) represents the upper middle borehole at Niche 3650, Yucca Mountain, before and after excavation Wang et al. (1999). (**b**) represents average permeability of N realizations of MPS simulated, conditioned to mean value of average permeability at 1.4×10^{-12} m^2 and permeability at top of drift surface

Table 2 Some basic THM rock properties used in Yucca Mountain simulation

Parameter	Yucca Mountaintype: volcanic tuff
Bulk density (kg/m^3)	2,370
Matrix porosity (–)	0.13
Young's modulus (GPa)	15
Poisson's ratio, (–)	0.21
Specific heat (J/kg°C)	985
Thermal conductivity (W/m°C)	2.29
Thermal expansion coefficient (°C^{-1})	1.0×10^{-5}
Bulk permeability (m^2)	3.3×10^{-13}

distribution of the observed fracture system can be found. Figure 11 shows a comparative result of water saturation between uniform and MPS simulated permeability. It can be seen that seepage repository drift in most cases (20 realizations) is much larger than that in the uniform permeability case. It indicates that fracture-induced heterogeneities in hydrological properties can increase the probability of seepage into opening, as they give rise to a

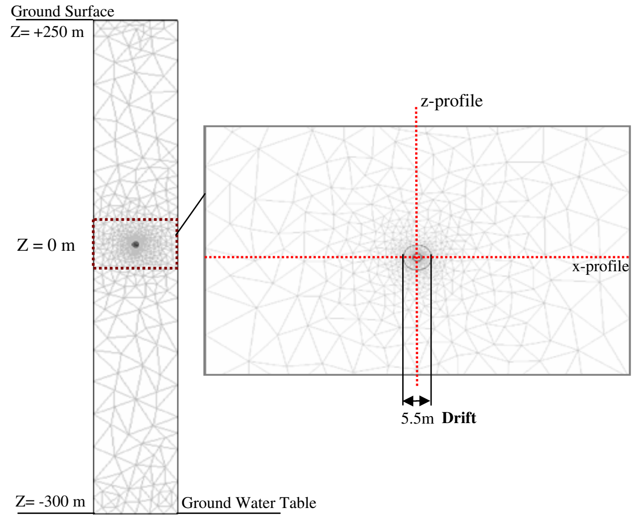


Fig. 9 Numerical grids and boundary conditions in simulation

considerable variation of saturation and capillary pressure in the unsaturated flow field. In this way, uncertainty in flow field simulation, even in complicated coupled THM simulation, can be evaluated statistically, like conventional stochastic theory. Meanwhile, MPS method has the advantage of reproducing the connectivity of known fracture observations. It can yield more real preferential pathway in water flow simulation.

Concluding remarks

In this study, a new method for fracture network description and prediction, termed multi-point-statistics (MPS) was introduced, which can classify and reconstruct pattern information from grid-based training image of discrete fracture network and was applied to fracture data from field observation to study flow field behavior in Yucca Mountain waste repository system. Flow field simulations were conducted considering two permeability distribution: uniform k, and MPS simulated k based on training image from filed database. The study shows that

1. Connectivity of fracture network in rock mass can be grasped and reconstructed by MPS method. In theory, it will lead to better prediction of fracture system characteristics and flow behavior prediction. It may show us where the water seepage is more probable to occur. Grid-based extrapolation is an important feather of multi-point-statistics which makes simulation flexible and less time-consuming when dealing with large-scale 2D/3D hydraulic problem.
2. Uncertainty in flow field simulation can be evaluated statistically by MPS method. It gives us a way to quantify both fracture pattern-induced heterogeneity in hydrological properties and uncertainty of stochastic

Fig. 10 Realizations of water saturation near repository drift (*squares* represent simulation area of near field around waste repository drift, 80 m × 80 m)

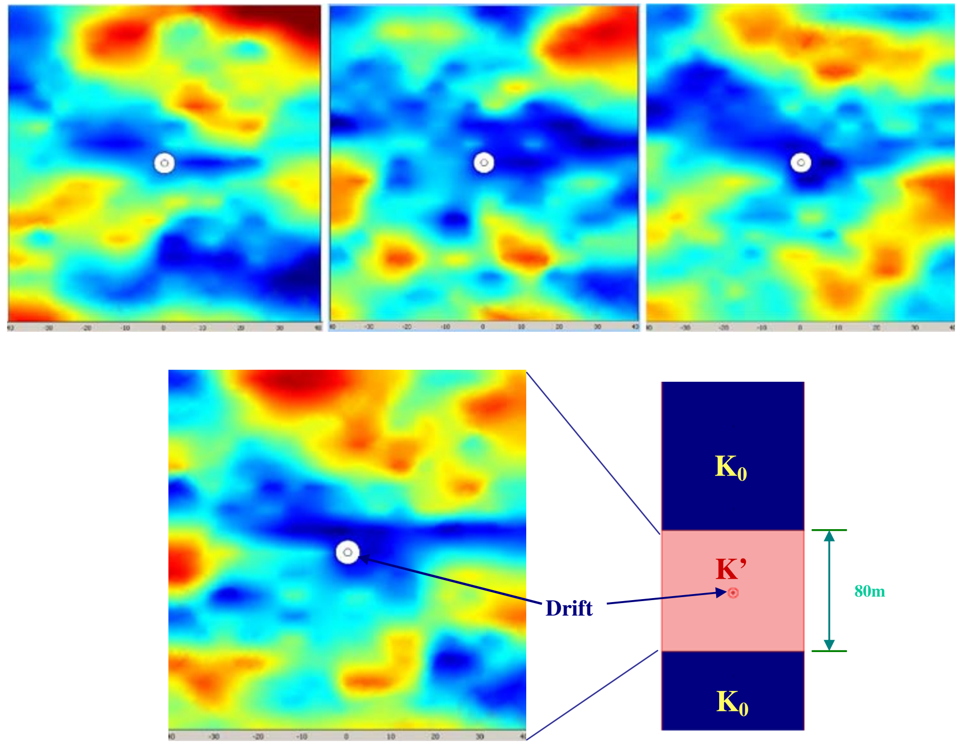
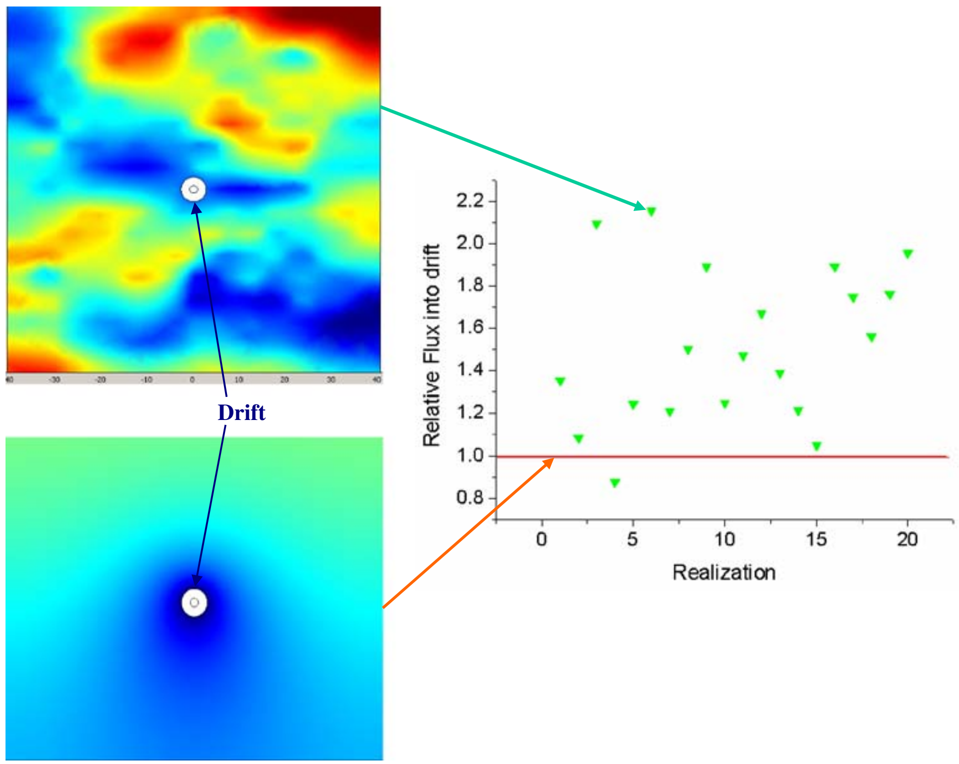


Fig. 11 Relative water seepage into repository drift with uniform and MPS simulated permeability (20 realizations, green triangle represents seepage into repository in one realization of simulated fracture network, *red line* represents seepage into repository in simulation with uniform permeability; *squares* at left represent simulation area near waste repository drift, 80 m × 80 m)



models simultaneously. This feature makes the MPS method superior to conventional fracture description methods. It is flexible when being used to evaluate uncertainty of stochastic models even in complicated coupled THM simulation.

This study indicates that multi-point statistical simulation is a potential method to characterize and reconstruct natural fracture network in a rock mass with capability of quantifying uncertainty in simulation. This is a preliminary study on fracture systems and their effect on flow fields.

The quantitative comparative study with conventional method is not considered here, but shall be carried out with conditioned data to measured Yucca Mountain drift seepage in further work. Moreover, different sources such as properly digitized outcrop or drift surface photographs or a geologist's sketch as training images should be used to combine more information for natural fracture networks and extend it to 3D case.

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