Modeling Scalar Variables on Unstructured Grids

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An outstanding issue in geostatistics research is the extension of modeling algorithms to unstructured grids, which are being used for reservoir flow analysis. Geostatistical algorithms are limited to regular grids; currently, models are built on a high resolution and upscaled to the flow grid. Several issues can be identified with this method. In various fields of computational mechanics and reliability analysis, where unstructured grids have been used for some time, accounting for uncertainty is becoming increasingly important. Methods are being developed that treat material properties as stochastic variables, a more prevalent one being the Karhunen-Loeve expansion. This series expansion technique represents a stochastic process as a series of orthogonal eigenvalues and eigenfunctions. It can be formulated independent of any mesh or grid (meshfree) and can be used to generate realizations of a stochastic process on unstructured grids intended for reservoir analysis. This preliminary paper on the subject covers the Karhunen-Loeve expansion, its meshfree formulation, and application to unstructured grids in geostatistics.

Introduction

Unstructured grids designed and used by reservoir analysts pose an interesting challenge for geostatistical modeling. The main use of the grids is to characterise flow of reservoir fluids with simulation to identify the potential of some recovery technique, be it traditional or enhanced. Therefore, grids are designed to conform to major reservoir structure such as horizons and faults, to capture a certain level of heterogeneity, and to obtain good accuracy of flow simulation results. Flow simulation requires these grids be characterized with reservoir properties, which is the purpose of geostatistics. However, geostatistical modeling algorithms are not designed with the same goals. They are intended to reproduce spatial heterogeneity and various statistics including the distribution and covariance. The targeted grids are pixel based and the algorithms cannot be used directly to characterize unstructured grids.

A very common and powerful geostatistical algorithm is sequential Gaussian simulation or SGS (Deutsch, 2002). It is based on the generation of Gaussian fields conditional to known information and with a specified covariance. Variables are treated as random point processes and realizations are generated over pixel based regular grids. These regular grids are typically of a higher resolution than unstructured grids. An upscaling procedure is used to assign property values to unstructured grid elements based on the SGS models (Farmer, 2002). The majority of references on upscaling target permeability due to its complexity and importance to flow; however, for any variable upscaling is essentially a numerical integration technique.

Therefore, an algorithm is required that retains the characteristics of SGS that has made it robust for quantification of uncertainty and that is applicable to unstructured grids. A similar problem has been encountered in mathematics with the description of physical processes that are controlled by partial differential equations. Examples include structural analysis, thermal convection, and fluid flow through porous media. All processes take place through materials such as a concrete beam, steel plate, or reservoir corresponding to the previous examples. For particular cases of these, it is more appropriate to treat the material properties as random – the distribution of grains in a concrete beam, thickness of a steel plate, or permeability throughout a reservoir can be considered uncertain in formulating the associated physical process. The stochastic finite element method (SFEM) has been devised for many of these types of problems (Ghanem and Dham, 1998; Eierman, Ernst, and Ullmann, 2007; Ghanem and Spanos, 2003). Several methods of generating random fields in SFEM exist; however, the most applicable that shares properties of SGS is to represent the random process as a series expansion. Expansion consists of a set of coefficients and functions that characterize a random process. A classical technique known as the Karhunen-Loeve (KL) expansion (Huang, Quek, and Phoon, 2001) produces a series that is bi-orthogonal: both the coefficients and functions are orthogonal. Therefore it is the most optimal representation of a random process (Hernandez, 1995).

KL expansion can generate fields with a given covariance function and is not restricted to any grid system making it well suited to geostatistical modeling of unstructured grids. In fact, the expansion problem can

be solved via meshfree methods: a relatively recent numerical scheme developed for computational mechanics (Nayroles, Touzot, and Villon, 1992; Liu and Gu, 2005). The remainder of this paper will discuss the issues with implementing SGS on unstructured grids. Also, a description of the KL expansion and its properties will be given along with the meshfree formulation of the expansion. The final section will describe how stochastic models can be generated for unstructured grids.

Background

SGS has several advantages for uncertainty quantification including the generation of models that reflect the heterogeneity throughout a reservoir and reproduction of the distribution and spatial correlation of sample data. The algorithm is stochastic in that several non-deterministic models can be generated, often referred to as a set of realizations. For reservoir decision making using flow simulation, realizations are processed to provide a distribution of performance measures. Unfortunately, SGS cannot be directly applied to unstructured grids. Instead, the algorithm is used to generate a set of realizations on a high resolution regular grid, which is upscaled to an unstructured grid. Several problems with this method exist:

1. Choosing the modeling scale, i.e. a representative elementary volume (REV) (Bear, 1972), for a regular grid is a non-trivial task. Rocks are heterogeneous at all scales. Reservoirs may contain large homogeneous regions that are overrepresented by the chosen scale while other areas may be much more heterogeneous than the chosen scale can represent. Choosing the finest scale would likely result in intractable models.
2. Regular grids will never exactly cover an unstructured grid (Figure 1). There will be an error term in the upscaling procedure used. This is especially hazardous for upscaling permeability, which typically involves solving the flow equations over the regular grid and integrating pressure and flux over the unstructured elements (Durlofsky, 2003).
3. Unstructured elements may represent a level of heterogeneity at a scale finer than the chosen regular grid scale. In this case, upscaling may assign a constant property value to all unstructured elements contained within a regular grid cell (Figure 2).
4. A wide variety of upscaling techniques for permeability exist, but their reliability is limited (Farmer, 2002). Both local and global methods exist, but results are dependent on boundary conditions, which must be chosen carefully to arrive at appropriate upscaled permeability.
5. For multiphase problems, upscaling of facies, hence rock curves, is not fully developed. It is commonly done with a majority vote average, which likely excludes important information from the reservoir (Zhang, Pickup, and Christie, 2005).

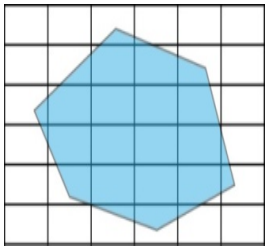

Figure 1: poor coverage of unstructured elements by regular grid

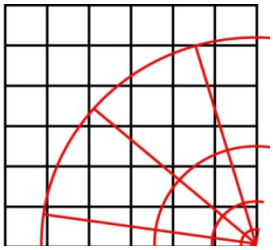

Figure 2: Unstructured grid with higher resolution than the regular grid

SGS is not restricted to regular grids and there is one possible extension for its direct application to unstructured grids. Instead of choosing a high resolution regular grid or REV, which omits problems 1 – 3, the upscaling of variables could be done dynamically (Manchuk and Deutsch, 2006). For an unstructured element, a number of points would be simulated, not necessarily on a regular grid, and upscaled. This numerical integration may be done according to some a priori error that is deemed acceptable, and integration points would be added until a lower error is achieved. Some issues still exist with this method including 4 and 5:

6. All integration points must be maintained during the generation of each realization to ensure the covariance is correct between them.

7. For a particular unstructured element, points cannot be added and simulated until enough are available for integration to achieve the specified error. Simulating points in clusters will introduce artefacts and poor variogram reproduction at ranges beyond the extents of the unstructured grid elements. Avoiding this issue requires all integration points be known a priori so they may be visited in a random sequence much like the existing SGS algorithms.
8. Depending on how integration points are chosen, traditional methods of upscaling permeability may not be applicable. Points will not form a regular grid and unstructured grid flow solvers will be required.

To avoid gridding issues, 1 – 3, 6 and 7, a technique for generating stochastic models independent of a grid system and other simulated points would be successful. The KL expansion shares the advantages of SGS and can be formulated with this latest condition.

Karhunen-Loeve Expansion

KL expansion is a series expansion technique that represents a stochastic process with an infinite series of deterministic functions (Hernandez, 1995). Other expansion techniques are possible, but the KL expansion gives an orthogonal series and hence an optimal representation of the stochastic process. Several assumptions are made about the stochastic process before defining the KL expansion, and all coincide with geostatistical applications. Assume the stochastic process $\omega(\mathbf{x})$ of spatial coordinate $\mathbf{x}$ is bounded by the domain Ω, has mean $\bar{\omega}(\mathbf{x})$ and finite variance $E[\omega(\mathbf{x})-\bar{\omega}(\mathbf{x})]^2$. Then the stochastic process can be represented by a series expansion (1) where λ_k and $f_k(\mathbf{x})$ are the eigenvalues and eigenfunctions of the covariance function, $C(\mathbf{x}_1, \mathbf{x}_2)$, of the stochastic process, and U is a series of random variables.

$$\omega(\mathbf{x}) = \bar{\omega}(\mathbf{x}) + \sum_{k=1}^{\infty} \sqrt{\lambda_k} U_k f_k(\mathbf{x}) \tag{1}$$

An additional assumption is the covariance function is bounded, symmetric, and positive definite – this is the case with covariance models defined in geostatistics. Determination of the eigenvalues and eigenfunctions is an integral equation problem (2).

$$\int_{\Omega} C(\mathbf{x}_1, \mathbf{x}_2) f_k(\mathbf{x}_2) d\mathbf{x}_2 = \lambda_k f_k(\mathbf{x}_1) \tag{2}$$

This is the Fredholm integral equation of the second kind (Atkinson, 1997). It is second kind because the function $f_k(\mathbf{x})$ to be determined is both inside and exterior to the integrand. Several methods exist to solve (2) and only certain covariance functions permit an analytical solution. A numerical method for multidimensional domains will be discussed in the following section. The solution results in an orthogonal set of eigenfunctions (3) and the random variables defined by (4) have zero mean and are uncorrelated (5). δ_{ij} is the Kroneker delta function defined by (6). The covariance function is reconstructed by Mercer's theorem (7) (Hernandez, 1995).

$$\int_{\Omega} f_i(\mathbf{x}) f_j(\mathbf{x}) d\mathbf{x} = \delta_{ij} \tag{3}$$

$$U_k = \frac{1}{\sqrt{\lambda_k}} \int_{\Omega} \left(\omega(\mathbf{x}) - \bar{\omega}(\mathbf{x}) \right) f_k(\mathbf{x}) d\mathbf{x} \tag{4}$$

$$\begin{aligned} E\left[U_k\right] &= 0 \\ E\left[U_i U_j\right] &= \delta_{ij} \end{aligned} \tag{5}$$

$$\delta_{ij} = \begin{cases} 1, \text{for } i = j \\ 0, \text{for } i \neq j \end{cases} \tag{6}$$

$$C(\mathbf{x}_1, \mathbf{x}_2) = \sum_{k=1}^{\infty} \lambda_k f_k(\mathbf{x}_1) f_k(\mathbf{x}_2) \tag{7}$$

Numerically, it is not practical to consider an infinite sum. Instead the series is truncated to a finite number of terms. This introduces a source of error, but it has been shown that the truncated expansion is mean square optimal (Hernandez, 1995; Ghanem and Spanos, 2003). For the special case where the stochastic process $\omega(\mathbf{x})$ is Gaussian, the vector U is a series of standard Gaussian values.

The preceeding description of the KL expansion is given in several other works including Hernandez (1995), Huang et al (2001), Ghanem and Spanos (2003), Phoon et al (2002[1,2], 2005), and Rahman and Xu (2005). Most references also suggest methods for solving (2); however, the more applicable method for multidimensional domains and any covariance kernel is the meshfree approach (Rahman and Xu, 2005; Liu and Gu, 2005).

Meshfree KL Expansion

Meshfree numerical simulation techniques are a recent development and Liu and Gu (2005) discuss several variations. Although the majority of references on meshfree methods are aimed at solving engineering problems described by partial differential equations, a formulation for the KL expansion has been explained by Rahman and Xu (2005). Unlike finite element methods (FEM) or finite volume methods (FVM) that involve discrete element or volumes, meshfree methods distribute a set of control points throughout the domain of interest based on some accuracy requirement or preprocessing. Each point has a local domain of support and there is no restriction on the interaction of multiple local domains (Figure 3). This is in contrast to FEM/FVM where elements do not intersect. Another notable difference is with interpolation of a variable within the domain. In FEM, interpolation is based on nodal values of an element containing the point, whereas in meshfree methods, interpolation is based on a set of control points in a local support domain of the point of interest. This technique has been termed a moving domain based interpolation by Liu and Gu (2005). This technique is very similar to kriging. Kriging interpolates the mean of a random variable based on surrounding conditioning data, which form the support domain.

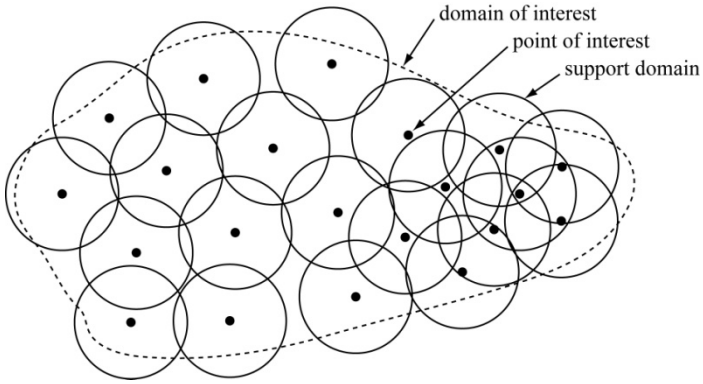

Figure 3: Circular support domains of points distributed through a domain of interest

Variables are interpolated using shape functions that depend on control points within a support domain. For the KL expansion, the eigenfunctions are interpolated at an arbitrary point in space based on (8), where $\mathbf{x}$ is the point location, m is the number of basis functions, $p_i(\mathbf{x})$ is a basis function, and $g(\mathbf{x})$ is a vector of coefficients to be determined. Shape functions to be developed are referred to as moving least squares (MLS) shape functions (Lancaster and Salkausdas, 1981). The coefficients are determined by minimizing the weighted squared difference, J, between $f_k(\mathbf{x}_i)$ and $\hat{f}_k(\mathbf{x})$ given by (9) where $\mathbf{x}_i$ is the i^{th} control point, $W(\mathbf{x}\text{-}\mathbf{x}_i)$ is a weight function that is non-zero in the support domain of $\mathbf{x}$, and N is the total number of control points. Note that the weight function beyond the local support domain of $\mathbf{x}$ is zero, so all N points in the sum are not necessary, but make notation more straightforward.

$$\hat{f}_k(\mathbf{x}) = \sum_{i=1}^{m} p_i(\mathbf{x}) g_{ik}(\mathbf{x}) = \mathbf{p}^T(\mathbf{x})\mathbf{g}_k(\mathbf{x}) \tag{8}$$

$$J = \sum_{i=1}^{N} W(\mathbf{x}-\mathbf{x}_i)\left[\mathbf{p}^T(\mathbf{x}_i)\mathbf{g}(\mathbf{x}) - f_k(\mathbf{x}_i)\right]^2 \tag{9}$$

Setting the partial derivative of J with respect to $\mathbf{g}$ to zero yields the following system of equations (10), where $\mathbf{A}(\mathbf{x})$ is defined by (11), $\mathbf{B}(\mathbf{x})$ by (12), and $\boldsymbol{F}$ is a vector of the values of $f_k(\mathbf{x})$ at control points.

$$\mathbf{A}(\mathbf{x})\mathbf{g}(\mathbf{x}) = \mathbf{B}(\mathbf{x})\mathbf{F} \tag{10}$$

$$\mathbf{A}(\mathbf{x}) = \sum_{i=1}^{N} W_i(\mathbf{x})\mathbf{p}(\mathbf{x}_i)\mathbf{p}^T(\mathbf{x}_i) \tag{11}$$

$$\mathbf{B}(\mathbf{x}) = \begin{bmatrix} W_1(\mathbf{x})\mathbf{p}(\mathbf{x}_1) & \cdots & W_N(\mathbf{x})\mathbf{p}(\mathbf{x}_N) \end{bmatrix} \tag{12}$$

Solving for $\mathbf{g}(\mathbf{x})$ and substituted back into (8) gives (13), which contains the definition of the MLS shape functions, $\boldsymbol{\Phi}(\mathbf{x})$. The i^{th} MLS shape function is defined by (14), where $\mathbf{B}_i(\mathbf{x})$ is the i^{th} column of $\mathbf{B}(\mathbf{x})$, or $W_i(\mathbf{x})\mathbf{p}(\mathbf{x}_i)$.

$$\hat{f}_k(\mathbf{x}) = \mathbf{p}^T(\mathbf{x})\mathbf{A}^{-1}(\mathbf{x})\mathbf{B}(\mathbf{x})\mathbf{F} = \boldsymbol{\Phi}^T(\mathbf{x})\mathbf{F} \tag{13}$$

$$\phi_i(\mathbf{x}) = \mathbf{p}^T(\mathbf{x})\mathbf{A}^{-1}(\mathbf{x})\mathbf{B}_i(\mathbf{x}) \tag{14}$$

The representation of $f_k(\mathbf{x})$ by a series of shape function can be substituted into the integral equation (2) which gives (15). This continuous operator equation can be formulated as a discrete one using Galerkin's method whereby the residual error defined by (16) is made orthogonal to the shape functions (17).

$$\sum_{i=1}^{N} \hat{f}_{ik} \int_{\Omega} C(\mathbf{x}_1, \mathbf{x}_2)\phi_i(\mathbf{x}_2)d\mathbf{x}_2 = \lambda_k \sum_{i=1}^{N} \hat{f}_{ik}\phi_i(\mathbf{x}_1) \tag{15}$$

$$\varepsilon = \sum_{i=1}^{N} \hat{f}_{ik} \left[\int_{\Omega} C(\mathbf{x}_1, \mathbf{x}_2)\phi_i(\mathbf{x}_2)d\mathbf{x}_2 - \lambda_k \sum_{i=1}^{N} \hat{f}_{ik}\phi_i(\mathbf{x}_1) \right] \tag{16}$$

$$\int_{\Omega} \varepsilon\phi_i(\mathbf{x})d\mathbf{x} = 0, \qquad i = 1, ..., m \tag{17}$$

Combining (16) with (17) yields (18), which is a generalized eigenvalue problem that can be formulated as (19) where $\mathbf{C}$ is defined by (20), $\mathbf{V}$ is an orthogonal matrix of eigenvectors, $\boldsymbol{\Lambda}$ is a diagonal matrix of eigenvalues, and $\mathbf{D}$ is defined by (21).

$$\sum_{i=1}^{N} \hat{f}_{ik} \int_{\Omega}\int_{\Omega} C(\mathbf{x}_1, \mathbf{x}_2)\phi_i(\mathbf{x}_1)\phi_j(\mathbf{x}_2)d\mathbf{x}_1 d\mathbf{x}_2 - \lambda_k \int_{\Omega} \phi_i(\mathbf{x})\phi_j(\mathbf{x})d\mathbf{x} = 0 \tag{18}$$

$$\mathbf{CV} = \boldsymbol{\Lambda}\mathbf{DV} \tag{19}$$

$$C_{ij} = \int_{\Omega}\int_{\Omega} C(\mathbf{x}_1, \mathbf{x}_2)\phi_i(\mathbf{x}_1)\phi_j(\mathbf{x}_2)d\mathbf{x}_1 d\mathbf{x}_2 \qquad i, j = 1, ..., N \tag{20}$$

$$D_{ij} = \lambda_k \int_{\Omega} \phi_i(\mathbf{x})\phi_j(\mathbf{x})d\mathbf{x} \qquad i, j = 1, ..., N \tag{21}$$

The solution to (19) provides the values at the meshfree control points. To obtain the k^{th} eigenfunction for any $\mathbf{x}$, the k^{th} column of $\mathbf{V}$ is assigned to $\mathbf{F}$ in (13), i.e. $\mathbf{F}_i = \mathbf{V}_{ik}$, $i = 1,\ldots,N$. Eigenvalues and eigenfunctions are substituted into (1) to generate the stochastic process with a covariance defined by $C(\mathbf{x}_1,\mathbf{x}_2)$.

In formulating (19), the most computationally demanding component is evaluating the integrals in (20) and (21). For a three dimensional problem, each ij element of $\mathbf{V}$ is a 6 dimensional integration and for $\mathbf{D}$ a 3 dimensional integration. Some simplifications are possible assuming the weight functions are zero beyond the local support domain of a point $\mathbf{x}$. D_{ij} will be zero for $\phi_i(\mathbf{x})$ and $\phi_j(\mathbf{x})$ that have an empty intersection (Figure 4). Also, V_{ij} will be zero when the local support domains of $\phi_i(\mathbf{x}_1)$ and $\phi_j(\mathbf{x}_2)$ are separated by more than the correlation length of $C(\mathbf{x}_1,\mathbf{x}_2)$ (Figure 5).

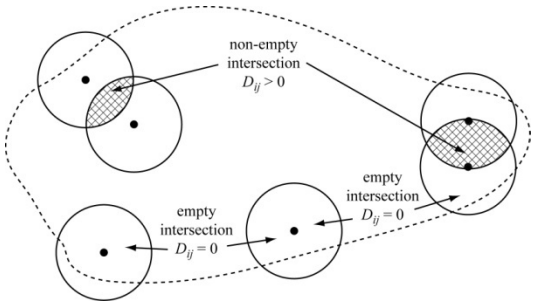

Figure 4: Reason for sparsity of D

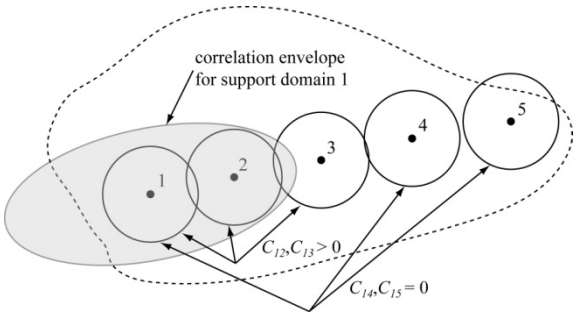

Figure 5: Reason for sparsity in C

Generating realizations

Like SGS, the formulation of a stochastic process via the KL expansion can be used to generate realizations. There is no dependence on an underlying grid however, which makes the later more attractive despite its upfront computational expense. Utilizing the KL expansion to generate a realization for an unstructured grid involves the following steps, assuming that a covariance function is already known for a variable of interest:

1. Choose basis functions and a weight function for the meshfree method. An example of basis functions is polynomials, much like for specifying a drift for SGS. Using 6 basis functions in two dimensions, $p^T(\mathbf{x}) = [1 \quad x \quad y \quad x^2 \quad xy \quad y^2]$. Choosing a weight function should be done such that the weight is positive within the domain of support, Ω^s, of a point $\mathbf{x}$, monotonically decreases away from $\mathbf{x}$ to zero at the boundary, $\partial\Omega^s$, of Ω^s, and is smooth on $\partial\Omega^s$ (Liu and Gu, 2005).
2. Discretize the domain containing the unstructured grid into a set of N control points. Points do not necessarily have to coincide with the unstructured grid discretization as the desired accuracy required to reproduce statistics of the stochastic process may be possible with far fewer. Using the same discretization would likely require different numerical methods to store and solve (19). Because unstructured grids are often designed to give higher accuracy where needed, it may be advantageous to use the same grid nodes for the meshfree KL expansion and obtain higher accuracy for the eigenfunctions in the same areas (Figure 6)
3. Build and solve (19) and choose a finite number, L, to truncate the series in (1). For a sufficiently large N, L may be increased while $L < N$ until acceptable covariance reproduction is achieved using (7).
4. Sample the stochastic process for any $\mathbf{x}$ within the unstructured grid by substituting (13) into (1), which gives (22). For a Gaussian field, $\mathbf{U}=[U_1,\ldots,U_N]$ is a standard Gaussian vector.

$$\begin{aligned} \omega(\mathbf{x}) &= \bar{\omega}(\mathbf{x}) + \sum_{k=1}^{L} \sqrt{\lambda_k} U_k \hat{f}_k(\mathbf{x}) \\ &= \bar{\omega}(\mathbf{x}) + \sum_{k=1}^{L} \sqrt{\lambda_k} U_k \boldsymbol{\Phi}^T(\mathbf{x}) \mathbf{F}_k \end{aligned} \tag{22}$$

5. If necessary, condition the result by kriging, which involves sampling the process at locations of conditioning data.

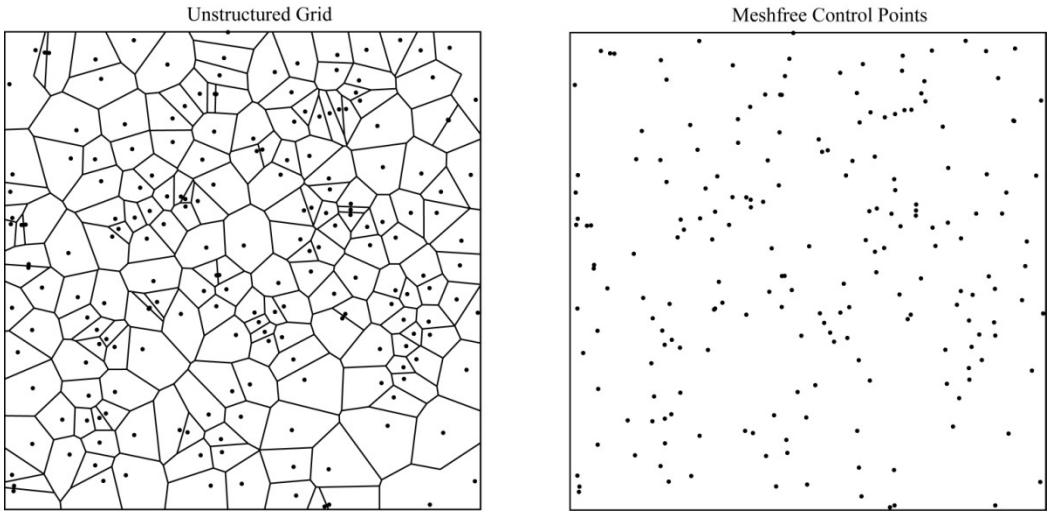

Figure 6: Unstructured grid and associated meshfree control points

In the 4th step, (22) can be written as a matrix equation involving all N eigenfunctions (23). Although this seems numerically demanding, $\mathbf{\Lambda}$ is diagonal simplifying its involvement and depending on the domain of support for $\mathbf{x}$, many entries in $\mathbf{\Phi}(\mathbf{x})$ may be zero.

$$\omega(\mathbf{x}) = \bar{\omega}(\mathbf{x}) + \mathbf{U}^T \mathbf{\Lambda}^{\frac{1}{2}} \mathbf{V}^T \mathbf{\Phi}(\mathbf{x}) \tag{23}$$

An advantage of (22) or (23) over SGS is realized when generating the stochastic process at multiple locations, $\mathbf{X} = [\mathbf{x}_1,\ldots,\mathbf{x}_n]$. There is no need to follow a random path to ensure covariance reproduction and there is no need to save previously simulated values. The concept of numerical integration over unstructured grid elements is more applicable and issues 1 – 3, 6, and 7 discussed in the background section can be omitted. Even though upscaling of permeability remains an issue, numerical integration of scalar variables such as porosity is possible. A number of quadrature rules are available (Kythe and Schaferkotter, 2004) and can be applied to unstructured grid elements. For a particular element Ω^e and a linear averaging scalar variable, the integral is given by (24).

$$\omega(\Omega^e) = \int_{\Omega^e} \bar{\omega}(\mathbf{x}) + \sum_{k=1}^{N} \sqrt{\lambda_k} U_k \mathbf{\Phi}^T(\mathbf{x}) \mathbf{F}_k d\mathbf{x} \tag{24}$$

Conclusion

The Karhunen Loeve expansion is an efficient method of storing the information contained in a stochastic process. It is being used more extensively in computational mechanics problems to deal with materials having random property distributions. Geostatistics involves the same idea where uncertainty is quantified by treating variables as random; however, it has been challenging to extending geostatistical tools to unstructured grids. This can be overcome by utilizing the KL expansion to generate realizations of reservoir properties. Its application to continuous scalar variables has been discussed and future developments involve facies or categorical variables and permeability or tensor variables. The expansion shares characteristics of sequential Gaussian simulation, including straightforward generation of Gaussian fields and reproduction of the covariance. It has an advantage in that a stochastic process can be sampled at any spatial location without explicitly ensuring the covariance between other samples is correct, i.e. previously simulated values are not necessary. This allows for a straightforward integration of scalar reservoir properties to unstructured grid elements.

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