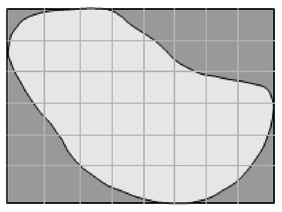
Quasi meshless discretization of random fields based on the Karhunen-Loève expansion



Master's thesis for the Master of Science program Computational Mechanics

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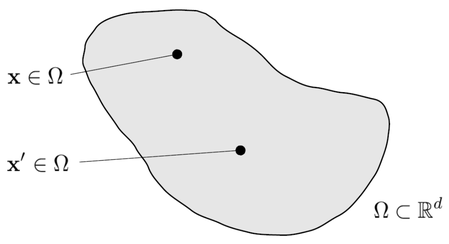
Abstract

A new quasi-meshless method for random field discretization with only a small number of random variables in the representation is introduced. The method is based on the Karhunen-Loève (KL) expansion, which is optimal among series expansion methods with respect to the mean square truncation error. The resulting integral eigenvalue problem in the KL-expansion is discretized using a finite cell (FC) like approach; i.e. the domain of computation is extended beyond the physical domain up to the boundaries of an embedding domain with a primitive geometrical shape. High order polynomials are used as FC shape functions.
The presented method is compared to the EOLE method. The EOLE method is considerably faster than the presented method in obtaining an approximation of a random field. However, working with the random field representation of the finite cell like approach is more efficient than EOLE in terms of computational costs.

Motivation

The Karhunen-Loève (KL) expansion is optimal in the mean square truncation error with respect to the number of random variables in the representation. However, its analytical solution is available only for a few autocovariance functions and geometries. For general geometries with a complex shaped domain a finite element based approach can be chosen to approximate the solution of the KL-expansion. However, this requires a spatial decomposition of the domain. Mesh generation for arbitrarily shaped domains can be a rather time-consuming task since in many cases it cannot be fully automated and manual work of the engineer is necessary. Moreover, the requirements for a good random field mesh are in general not the same as the requirements for a good mesh modeling the corresponding mechanical system.
A quasi-meshless approach is to embed the physical domain in a larger domain of primitive geometrical shape which can be meshed easily. The shape functions are spanned on the embedding fictitious domain. The actual physical domain is taken into account through integration because the functions to integrate are considered to be zero outside of the physical domain. This is the idea of the finite cell method which shifts the problem with complex geometries from the mesh to the integration.
The present work applies a finite cell like approach to discretize the spatial domain of the random field and to solve the KL-expansion numerically. The behavior of the proposed method is compared to the EOLE method which is considered an efficient method and is well applied in practice.

Random Field



A *continuous real-valued random filed* $\mathrm{H}(\mathbf{x})$ may be loosely defined as a random function which describes a random variable (RV) at each point $\mathbf{x}$ of a continuous domain Ω. A *Gaussian* random field can be completely defined by its mean function $\mu(\mathbf{x})$ and autocovariance function $\mathrm{Cov}(\mathbf{x},\mathbf{x}')$. The autocovariance function is expressed in terms of the autocorrelation coefficient function $\rho(\mathbf{x},\mathbf{x}')$ as:

$$\mathrm{Cov}(\mathbf{x},\mathbf{x}')=\sigma(\mathbf{x})\cdot\sigma(\mathbf{x}')\cdot\rho(\mathbf{x},\mathbf{x}')$$

where $\sigma(\mathbf{x})$ is the standard deviation function of the random field (RF).

Discretization

A random field consists of an infinite number of random variables. For computational purposes a random field has to be expressed using a finite number M of random variables; this is referred to as *random field discretization*. A random field discretization method is said to be efficient if it accurately represents a random field with only a small number of RVs.

Error variance

Different error measures can be used to assess the quality of a random field discretization. The difference between the original RF and its approximation is known as truncation error $\varepsilon_{\mathrm{H}}(\mathbf{x})$.

$$\bar{\varepsilon}_{\sigma}(\mathbf{x})=\frac{\mathrm{Var}\left(\mathrm{H}(\mathbf{x})-\hat{\mathrm{H}}(\mathbf{x})\right)}{\mathrm{Var}\left(\mathrm{H}(\mathbf{x})\right)}$$

The variance of the truncation error weighted by the variance of the original field is referred to as *error variance* $\varepsilon_{\sigma}(\mathbf{x})$.

$$\bar{\varepsilon}_{\sigma}(\mathbf{x})=\frac{\int_{\Omega}\varepsilon_{\sigma}(\mathbf{x})\mathrm{d}\,\mathbf{x}}{|\Omega|}$$

The *mean error variance* is defined as the integral of the error variance over the domain weighted by the absolute value of the domain.

Karhunen-Loève expansion

The *Karhunen-Loève (KL) expansion* is a method for representing a random field $\mathrm{H}(\mathbf{x})$ based on the spectral decomposition of its autocovariance function. The expansion writes:

$$\mathrm{H}(\mathbf{x},\boldsymbol{\xi})=\mu(\mathbf{x})+\sum_{i=1}^{\infty}\sqrt{\lambda_i}\cdot\varphi(\mathbf{x})\cdot\xi_i$$

where the ξ_i's are independent standard Gaussian random variables, and λ_i and $\varphi_i(\mathbf{x})$ are the eigenvalues and eigenfunctions of the autocovariance function.

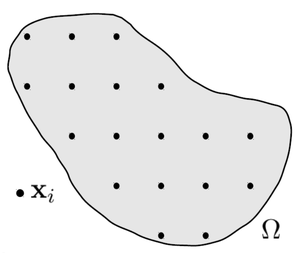
The eigenpairs $[\lambda_i, \varphi_i(\mathbf{x})]$ can be obtained by solving the following integral eigenvalue problem:

$$\int_{\Omega'}\mathrm{Cov}(\mathbf{x},\mathbf{x}')\cdot\varphi_i(\mathbf{x}')d\mathbf{x}'=\lambda_i\cdot\varphi_i(\mathbf{x}) \qquad \forall i=1,2,\ldots$$

Ordering the eigenpairs w.r.t. the magnitude of the eigenvalues in a descending series and truncating it after M terms gives an approximation (discretization) of the random field:

$$\hat{\mathrm{H}}(\mathbf{x},\boldsymbol{\xi})=\mu(\mathbf{x})+\sum_{i=1}^{M}\sqrt{\lambda_i}\cdot\varphi(\mathbf{x})\cdot\xi_i \qquad \bar{\varepsilon}_{\sigma}(\mathbf{x})=1-\frac{1}{\sigma^2|\Omega|}\sum_{i=1}^{M}\lambda_i$$

EOLE method



In the*EOLE (expansion optimal linear estimation) method* the random field is discretized using a finite number of points. In a first step, the points to discretize the field have to be chosen. Thereafter, the covariance matrix of the random variables υ_i at the chosen points $\mathbf{x}_i$ is computed, $(\Sigma_{\upsilon\upsilon})_{nm}=\mathrm{Cov}(\mathbf{x}_n,\mathbf{x}_m)$. In a next step, the eigenvalues θ_i and eigenvectors $\boldsymbol{\Phi}_i$ of the covariance matrix are computed. Only the M largest eigenvalues and their corresponding eigenvectors are selected for the random field discretization. The EOLE method does not require a mesh since the geometry of the domain is considered indirectly through the points used to discretize the field.

The expansion writes:

$$\hat{\mathrm{H}}(\mathbf{x},\boldsymbol{\xi})=\mu(\mathbf{x})+\sum_{i=1}^{M}\frac{\boldsymbol{\Phi}_i^{\mathrm{T}}\boldsymbol{\Sigma}_{\upsilon\mathbf{x}}(\mathbf{x})}{\sqrt{\theta_i}}\cdot\xi_i$$

where the vector function $\boldsymbol{\Sigma}_{\upsilon\mathbf{x}}(\mathbf{x})$ is defined as $(\boldsymbol{\Sigma}_{\upsilon\mathbf{x}}(\mathbf{x}))_j=\mathrm{Cov}(\mathbf{x}j,\mathbf{x})$, and the ξ_i are independent standard normal random variables.

The expansion was set-up such that it minimizes the variance of the truncation error at the discretization points subjeted to a zero mean truncation error.

$$\varepsilon_{\sigma}(\mathbf{x})=1-\frac{1}{\sigma^2}\sum_{i=1}^{M}\frac{\left(\boldsymbol{\Phi}_i^{\mathrm{T}}\boldsymbol{\Sigma}_{\upsilon\mathbf{x}}(\mathbf{x})\right)^2}{\theta_i}$$

pFEM - Karhunen-Loève

The integral eigenvalue problem of the KL-expansion can be solved analytically only for few autocovariance functions and geometries. For general problems a computational approach is necessary. This involves a discretization of the integral eigenvalue problem, and introduces yet another approximation to the representation of the RF. This approach is referred to as *pFEM-KL*.

The eigenfunctions are approximated as:

$$\hat{\varphi}_i(\mathbf{x})=\sum_{n=1}^{N}\mathbf{d}_n^i\cdot\mathrm{N}_{\mathrm{n}}(\mathbf{x})$$

where N is the number of shape functions, $\mathrm{N}_n(\mathbf{x})\in L^2(\Omega)$ are the global shape functions and d^i_n are the coordinates of the ith eigenfunction in the basis spanned by the shape functions.

The approximated integral eigenvalue problem can be written as:

$$\int_{\mathbf{x}'\in\Omega}\hat{\varphi}_i(\mathbf{x}')\mathrm{Cov}(\mathbf{x},\mathbf{x}')\,\mathrm{d}\,\mathbf{x}'-\lambda_i\,\hat{\varphi}_i(\mathbf{x})=\tilde{\varepsilon}_N^i(\mathbf{x})$$

where the term on the right-hand side is the error resulting from the approximation of the eigenfunction.

$$\left\langle\tilde{\varepsilon}_N^i,\mathrm{N}_k\right\rangle_{L^2(\Omega)}=0$$

Using a Galerkin scheme the coefficients d^i_n are determined such that the error term becomes orthogonal to the subspace spanned by the shape functions. The eigenfunctions must be scaled to be orthonormal.

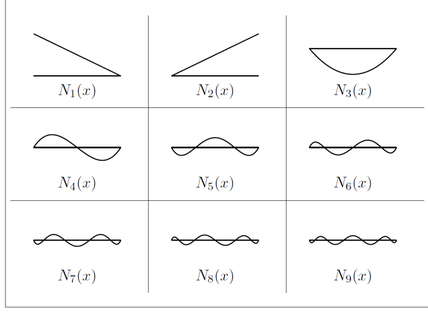
The solution is the following general matrix eigenvalue problem: $\mathbf{B}\mathbf{d}_i=\lambda_i\mathbf{M}\mathbf{d}_i$

The coefficients of the matrices $\mathbf{B}$ and $\mathbf{M}$ are defined as:

$$\mathbf{B}_{kn}=\int_{\mathbf{x}\in\Omega}\mathrm{N}_k(\mathbf{x})\int_{\mathbf{x}'\in\Omega}\mathrm{N}_k(\mathbf{x}')\mathrm{Cov}(\mathbf{x},\mathbf{x}')\,\mathrm{d}\,\mathbf{x}'\,\mathrm{d}\,\mathbf{x} \qquad \mathbf{M}_{ij}=\int_{\mathbf{x}\in\Omega}\mathrm{N}_i(\mathbf{x})\,\mathrm{N}_j(\mathbf{x})\,\mathrm{d}\,\mathbf{x}$$

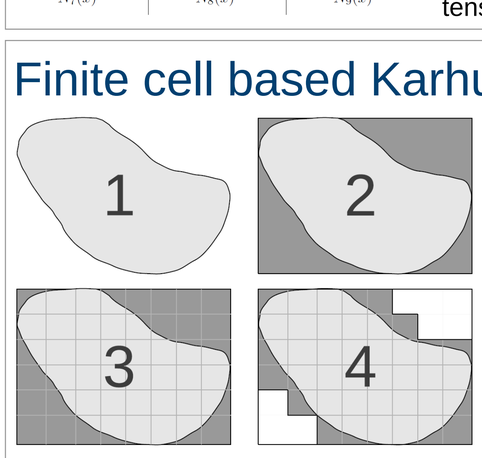
The mean error variance is defined by the same equation as in case of the analytical Karhunen-Loève expansion.

Hierarchic basis



In this work a hierarchic basis based on the Legendre polynomials is chosen as Ansatz space for the shape functions. The first nine one-dimensional polynomials of this space are depicted on the left. Two- and three-dimensional spaces can be constructed by combining the one-dimensional polynomials for the different coordinate directions with each other. In a two-dimensional setting this results in nodal-, edge- and face-modes. For the face-modes two different ways of combining the one-dimensional polynomials are investigated: *tensor-space* and *trunk-space*, where trunk-space is a sub-space of tensor-space (see [1] for a more detailed description).

Finite cell based Karhunen-Loève (FC-KL)



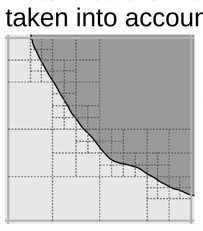
To overcome the problem of meshing geometrically complex shaped domains, the physical domain Ω *(1)* is embedded in a larger fictitious domain Ω^* having a geometrically primitive shape *(2)*. The fictitious domain can be meshed easily *(3)*; the elements of this mesh are called finite cells. Consequently, the shape functions $\mathrm{N}_n(\mathbf{x})\in L^2(\Omega^*)$ are spanned over the fictitious domain. Cells completely outside of the physical domain are neglected since they do not contribute to the solution *(4)*.

$$\alpha(\mathbf{x})=\begin{cases}1 & \forall\mathbf{x}\in\Omega\\ 0 & \forall\mathbf{x}\in\Omega^*\setminus\Omega\end{cases}$$

Using the factor $\alpha(\mathbf{x})$, the coefficients of the matrix eigenvalue problem $\mathbf{B}\mathbf{d}_i=\lambda_i\mathbf{M}\mathbf{d}_i$ become:

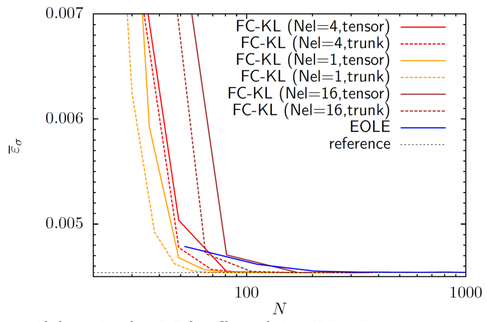
$$\mathbf{B}_{kn}=\int_{\mathbf{x}\in\Omega}\alpha(\mathbf{x})\,\mathrm{N}_k(\mathbf{x})\int_{\mathbf{x}'\in\Omega}\alpha(\mathbf{x}')\,\mathrm{N}_k(\mathbf{x}')\mathrm{Cov}(\mathbf{x},\mathbf{x}')\,\mathrm{d}\,\mathbf{x}'\,\mathrm{d}\,\mathbf{x} \qquad \mathbf{M}_{ij}=\int_{\mathbf{x}\in\Omega}\alpha(\mathbf{x})\,\mathrm{N}_i(\mathbf{x})\,\mathrm{N}_j(\mathbf{x})\,\mathrm{d}\,\mathbf{x}$$

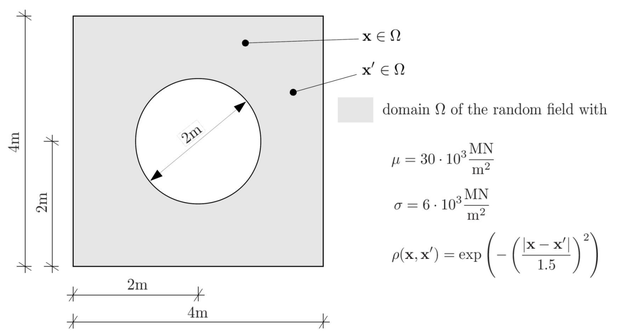
Note that the integral is computed on the fictitious domain, although only the physical domain is taken into account because of the factor $\alpha(\mathbf{x})$.



Due to the discontinuity in $\alpha(\mathbf{x})$, the functions to integrate become discontinuous at the boundary of the physical domain. Therefore, special numerical integration techniques have to be applied. In the context of this work, the cells cut by the boundary of the physical domain are refined in a tree-based manner, and Gaussian integration is performed for the sub-cells. The sub-cells cut by the boundary of the physical domain are treated specially by taking the physical shape of their physical sub-domain into account.

Results





In this study M is fixed to 20. FC-KL was investigated for meshes with 1x1, 2x2 and 4x4 elements. The mean error variance is plotted for an increasing size N of the eigenvalue problem. The best convergence was achieved with FC-KL on a 1x1 mesh and trunk-space. However, FC-KL was computationally significantly more expensive to solve than the corresponding EOLE-problem.

In a next step the obtained random field representations were used to model the random behavior of the Young's modulus in a structural finite element (FE) problem. A significant speed-up of the time needed to assemble and solve the FE-problem was observed for FC-KL compared to EOLE. In this case no advantageous behavior of trunk-space over tensor-space could be detected.

Conclusion

Both FC-KL and EOLE are meshless approaches. The FC-KL method is difficult to implement and quite expensive to solve compared to the EOLE method. Numerical problems w.r.t. the eigenvalue problem to solve may arise.
Compared to the EOLE method, FC-KL has shown to be more efficient for post-processing the random field because it computes a realization of the field faster than EOLE. This is especially useful if the random field is used as input for finite element problems where the problem must be solved several times for different random field realizations.

References

[1] Wolfgang Betz: Quasi meshless discretization of random fields based on the Karhunen-Loève expansion, Master's thesis, ERA Group, Fakultät Bauingenieurwesen, TU München, 2012