On sampling spatially-correlated random fields for complex geometries

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Motivations

The ubiquitous presence of **tissue heterogeneities** affects the electrophysiological and mechanical function of the heart. The severity of these effects is clearly seen in the **atria**, for instance.

Heterogeneities are hard or impossible to extract from clinical imaging. An alternative is to include such heterogeneities as **random variables**, reflecting the lack of knowledge of local tissue properties.

Standard methods to generate spatially-correlated random fields are not suitable for **complex geometries**. Here we propose two approaches, based on: stochastic PDEs, and a modification of Karhunen-Loève expansion.

Methods

Random fields via Karhunen-Loève with geodesic distance (geoKL)

▶ **Random fields via Karhuhen-Loève (KL) expansion.**

Given a square-integrable correlation function $r(x,y)$, the random field $u(x,\omega)$ with mean $\bar{u}(x)$ and covariance $r(x,y)$ reads as follows:

$$u(x,\omega) = \bar{u}(x) + \sum_{i=1}^{\infty} \sqrt{\lambda_i}\psi_i(x) Z_i(\omega), \qquad Z_i \text{ i.i.d. } \mathcal{N}(0,1),$$

where $\{\lambda_i\}$ and $\{\psi_i\}$ are respectively eigenpairs of the problem (in discrete setting):

$$\mathbf{A}\mathbf{v} = \lambda \mathbf{M}\mathbf{v}, \qquad [\mathbf{A}]_{ij} = \int_\Omega \int_\Omega r(x,y)\phi_j(y)\phi_i(x)\,\mathrm{d}x\mathrm{d}y.$$

▶ **What if the problem is large?**

With the low-rank pivoted Cholesky decomposition we can efficiently approximate the (large) matrix $\mathbf{A} \in \mathbb{R}^{N\times N}$ by the low-rank matrix $\mathbf{A}_m := \mathbf{L}_m \mathbf{L}_m^\mathrm{T}$, with $\mathbf{L}_m \in \mathbb{R}^{N\times m}$, $m \ll N$ and such that $\|\mathbf{A} - \mathbf{A}_m\| < \varepsilon$. For short-length correlation kernels $\mathcal{H}$-matrices are preferable.

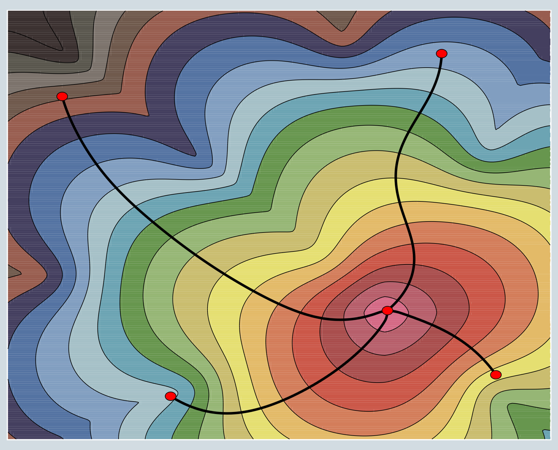
▶ **How to account for the geometry of the domain?**

We define the correlation kernel as function of **geodesic distance**: therefore, geometrically-close but topologically distinct regions correctly show small correlation.

$$r(x,y) = h\big(\delta(x,y)\big),$$

where

$$\delta(x,y) = \text{shortest distance between } x \text{ and } y.$$



We can also model non-stationary and anisotropic fields just by changing the metric in the eikonal equation.

▶ **Isn't it too expensive to compute?**

The low-rank pivoted Cholesky algorithm only needs the diagonal entries and the function returning the i-th row of the matrix. Therefore, for fixed row i, we set

$$h\big(\delta(x,y)\big) \approx h\big(\delta(x_i,y)\big)$$

where $\delta(x_i,y)$ is the solution of the **eikonal equation**. The number of eikonal evaluations matches the rank of $\mathbf{A}_m$.

▶ **Drawbacks?**

It is possible that a specific combination of kernel and distance yields an indefinite Hilbert-Schmidt operator.

Random fields sampled via Stochastic PDEs (SPDEs)

▶ **PDE as sampling tool.**

A simple, yet powerful method to sample random fields on arbitrarily complex geometries is based on SPDEs. We consider the following one:

$$\begin{cases} (\kappa^2 - \nabla\cdot\mathbf{D}\nabla)^{\frac{\alpha}{2}} u = \mathcal{W}, & x \in \Omega \subset \mathbb{R}^d, \\ \mathbf{D}\nabla(\kappa^2 - \nabla\cdot\mathbf{D}\nabla)^j \cdot \mathbf{n} = 0, & x \in \partial\Omega,\ j = 0,\dots,\left\lfloor\frac{\alpha-1}{2}\right\rfloor. \end{cases}$$

where

– $\kappa > 0$ is inversely proportional to the correlation length;
– $\alpha = \nu + d/2$, d dimension and $\nu > 0$ is a measure of the smoothness of the random field;
– $\mathbf{D}(x)$ is a uniformly elliptic tensor field;
– $\mathcal{W}$ Gaussian white noise.

An explicit link between this SPDE and random fields with Matérn kernel was established by Lindgren *et al.* (2011).

▶ **How to solve the fractional SPDE?**

The solution for general α is tricky, but when $\alpha/2 = K \in \mathbb{N}$, which corresponds to the choice $\nu = 2K - d/2$, an iterative scheme applies.

$$u_0 = \mathcal{W}, \quad \begin{cases} (\kappa^2 - \nabla\cdot\mathbf{D}\nabla)u_k = u_{k-1}, & x \in \Omega,\ k = 1,\dots,K, \\ \mathbf{D}\nabla u_k \cdot \mathbf{n} = 0, & x \in \partial\Omega,\ k = 1,\dots,K. \end{cases}$$

In the discrete setting, the algorithm reduces to:

$$\begin{cases} \mathbf{K}\mathbf{u}_1 = \mathbf{w}, \\ \mathbf{K}\mathbf{u}_k = \mathbf{M}\mathbf{u}_{k-1}, & k = 2,\dots,K, \end{cases}$$

where $\mathbf{w}$ is the discrete Gaussian white noise, that is an N-dimensional Gaussian sample with zero mean and covariance $\mathbf{M}$.

▶ **How to sample white noise on general domains?**

Efficient methods to sample the discretized white noise have been proposed.

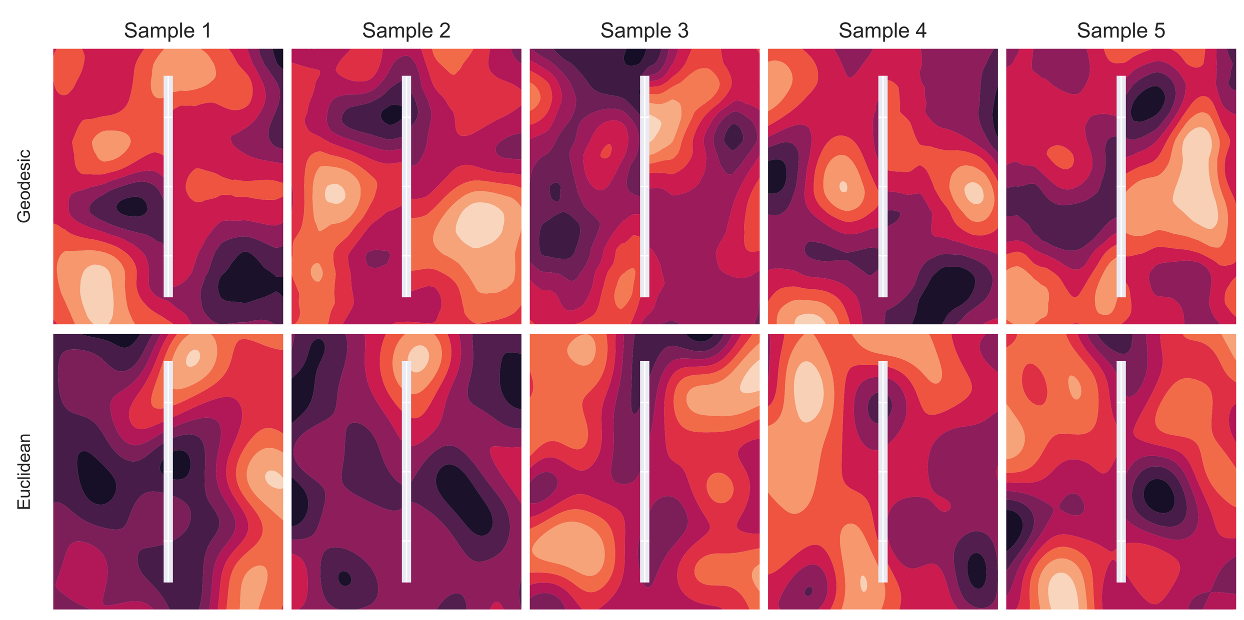
– **Mass lumping**: easy for linear finite elements, but not for higher-order polynomials.
– Croci *et al.*: **element-wise** Cholesky decomposition of the mass matrix, evaluation of white noise very efficient and parallelizable.
– Galerkin space V_h with an **orthonormal basis**, as for instance in spectral methods.

▶ **Drawbacks?**

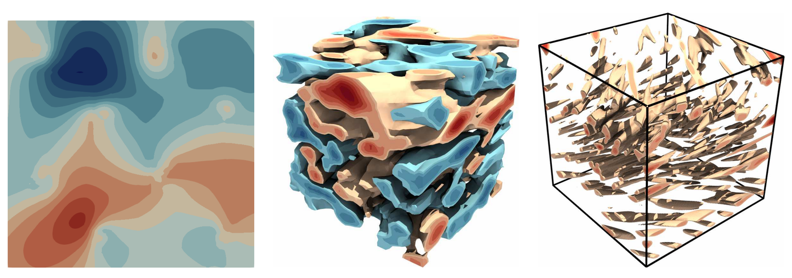
Correlation implicitly defined through the parameters of the PDE.
Each sample requires the solution of a linear system.

Results

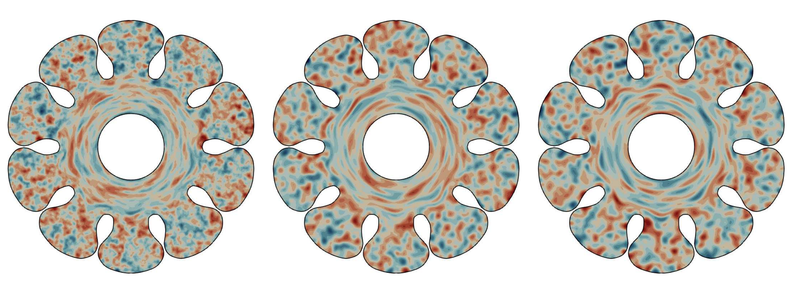
Examples



Random fields with covariance $r(x,y) = e^{-(d(x,y)/\rho)^2}$ sampled via geoKL with $d(x,y)$ either geodesic or Euclidean ($\rho = 0.2$).

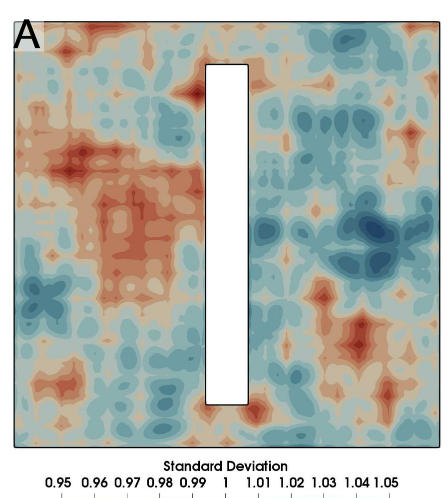


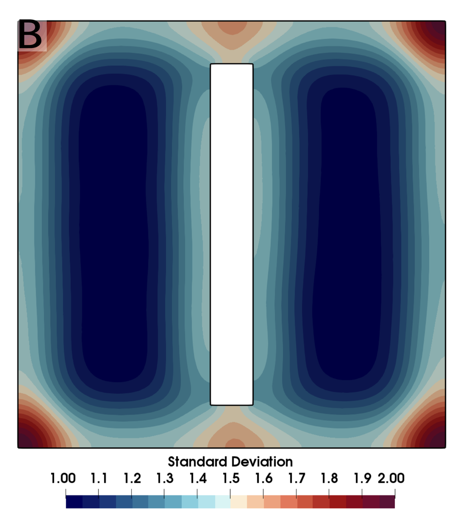
Non-stationary random field in 2D and 3D with mild and strong anisotropy using geoKL.

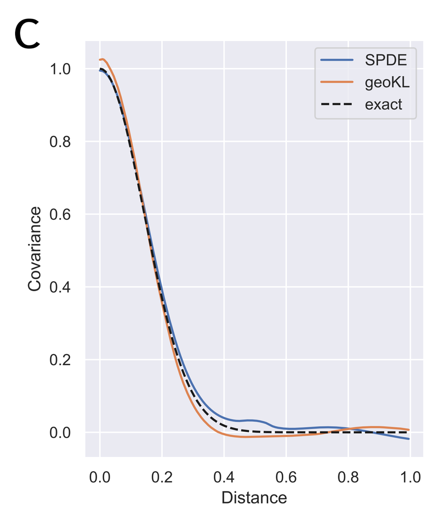


Non-stationary and anisotropic random fields with SPDE, increasing value of ν from left to right.

Comparison





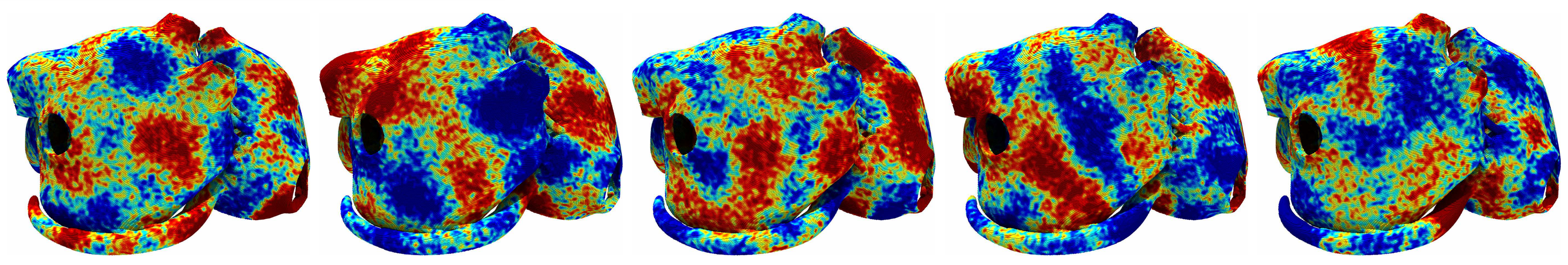


$N = 10\,000$ samples defined on a hollow square domain, uniform mesh $h = 1/100$, squared-exponential kernel $h(d) = e^{-d^2/\rho^2}$ in geoKL with $\rho = 0.2$ and $K = 5$, $\kappa = 2\sqrt{\nu}/\rho$ in SPDE.

GeoKL: error in variance uniform with some oscillations due to approximate geodesic distance (Figure A).
Cost: 26 s setup, negligible per sample.

SPDE: strong boundary effect in the variance, being significantly larger close to the boundary (Figure B).
Cost: no setup, 3 s per sample.

Application 1: Atrial Fibrosis



Random fibrosis patterns, superposition of coarse-scale field ($\rho = 2$ cm) and fine-scale field ($\rho = 2$ mm).

Application 2: Uncertainty Quantification

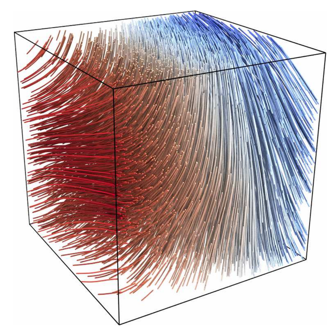
Methodology successfully applied to study the effect of randomly perturbed fiber field in electrophysiology:

$$\alpha(x,\omega) = \alpha_0(x) + \sum_{i=1}^{\infty} \sqrt{\lambda_i}\psi_i(x) Z_i(\omega), \qquad Z_i \text{ i.i.d. } \mathcal{N}(0,1),$$

where $\alpha_0(x)$ is the fiber angle with the usual rule-based rotation.

Applied in UQ with:

▶ Multi-Level Monte Carlo (MLMC): hierarchy of grids, most of samples drawn on coarsest grid.
▶ Multi-Fidelity Monte Carlo (MFMC): hierarchy of models, eikonal and bidomain.



Final Remarks

We presented two alternative approaches to simulate spatially-correlated random fields for complex geometries. A potential application of such techniques is the automatic generation of realistic fibrosis patterns for the atria. Uncertainty-aware cardiac simulation should become fundamental in view of clinical application.

Quaglino A., Pezzuto S., Krause R.. High-dimensional and higher-order multifidelity Monte Carlo estimators. *J Comp Phys* Vol. 388, 2019, Pages 300-315.

Pezzuto S., Gharaviri A., Schotten U., Potse M., Conte G., Caputo M.L., Regoli F., Krause R., Auricchio A.. Beat-to-beat P-wave morphological variability in patients with paroxysmal atrial fibrillation: an in silico study. *EP Europace*, Vol. 20(suppl_3), 2018, Pages iii26-iii35.

Would like to try to generate random fields yourself? Try out the code here: `https://github.com/pezzus/fimh2019`.

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