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Effects of Inhomogeneity and Anisotropy on THM Simulations

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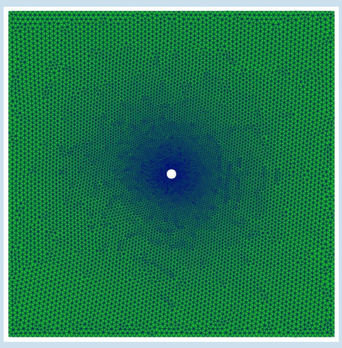
Motivation and highlights

- Barrier integrity investigations
- Applications such as nuclear waste disposal
- Coupled THM numerical simulations using OpenGeoSys-6
- Accounting for uncertainty in input parameters
- Effects of transverse anisotropy of input parameters
- Input parameters as heterogeneous random fields

Model setup and specifics

- Simplified 2D mesh based on FE experiment [Müller et al. 2018]
- host rock (Opalinus clay) –> $100\,\mathrm{m} \times 100\,\mathrm{m}$
- Circular heat source of $3\,\mathrm{m}$ diameter –> emplaced waste cell
- Anisotropic –> Transverse isotropy –> parallel and perpendicular to bedding plane
- Heterogeneous input parameters –> Random fields generation with `kleme`
- Uncertainty quantification using numerical modeling –> ThermoRichardsMechanics (TRM) –> OpenGeoSys-6
- Comparison of results with homogeneous, isotropic models



Initial conditions:
$T_0 = 15\,°\mathrm{C}$, $p_0 = 2\,\mathrm{MPa}$, $u_{S0} = 0$
Boundary conditions:

- Q_T (Neumann) at tunnel boundary
- $p = 0$ at tunnel boundary
- Normal $u_S = 0$ on outer boundary

Generation of random fields through the `kleme` library

- The permeability field is assumed to be log-Gaussian;
- Realizations of Gaussian random fields are generated by the truncated Karhunen-Loève expansion, which approximates a random field as

$$\mathbf{Z}(\mathbf{x}, \xi) \approx \overline{\mathbf{Z}}(\mathbf{x}) + \sum_{i=1}^{M} \xi_i \sqrt{\lambda_i} \mathbf{f}_i(\mathbf{x})$$

where $\overline{\mathbf{Z}}(\mathbf{x})$ is the mean of the field, $\{\xi_i\} \sim \mathcal{N}(0,1)$, and $\{\mathbf{f}_i\}$ and $\{\lambda_i\}$ are eigenfunctions and eigenvalues of the covariance operator

$$(Cu)(\mathbf{x}) = \int_D c(\mathbf{x}, \mathbf{y}) u(\mathbf{y}) \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{y}$$

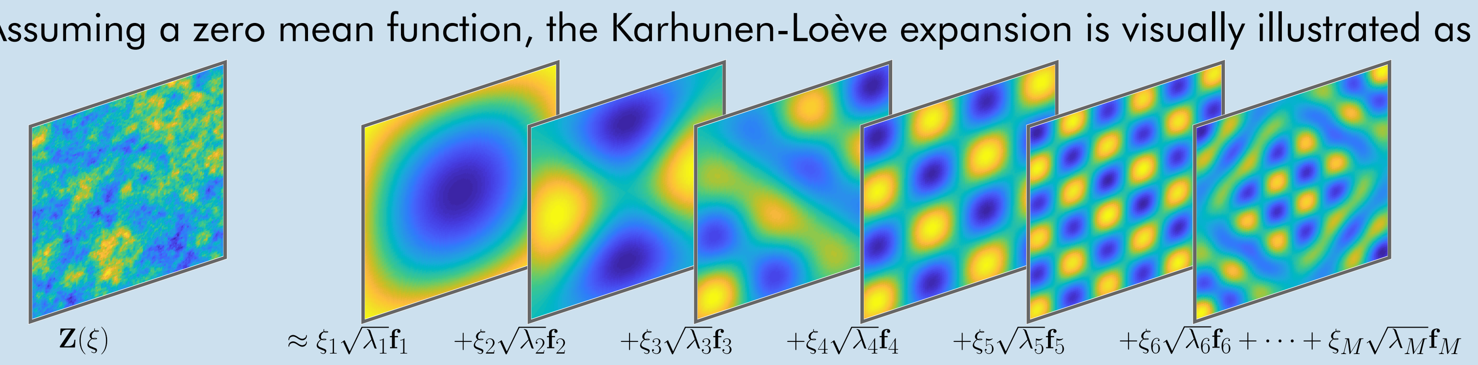
and $c(\mathbf{x}, \mathbf{y})$ is the covariance function;

- The Galerkin method is used to discretize the covariance operator and then solve for the eigenfunctions and eigenvalues;
- The exponential covariance function is used in this study

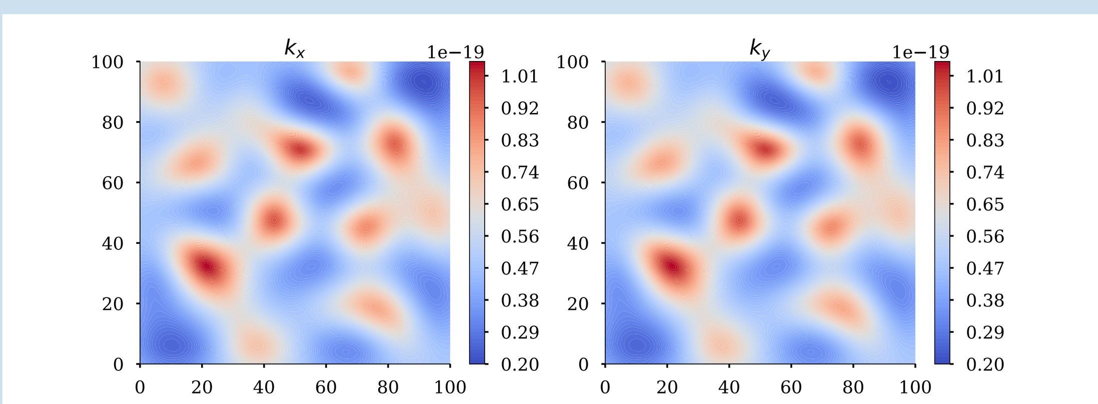
$$c(\mathbf{x}, \mathbf{y}) = \sigma^2 \exp\left(-\frac{|(\mathbf{x} - \mathbf{y})|}{l}\right)$$

where σ is the scale factor and l is the correlation length;

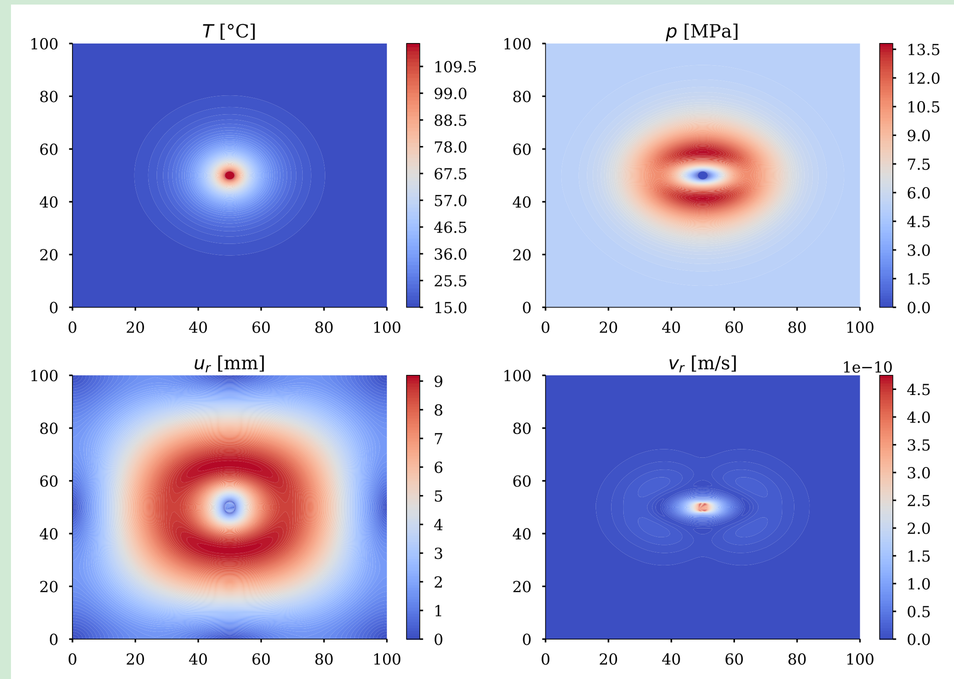
- Assuming a zero mean function, the Karhunen-Loève expansion is visually illustrated as



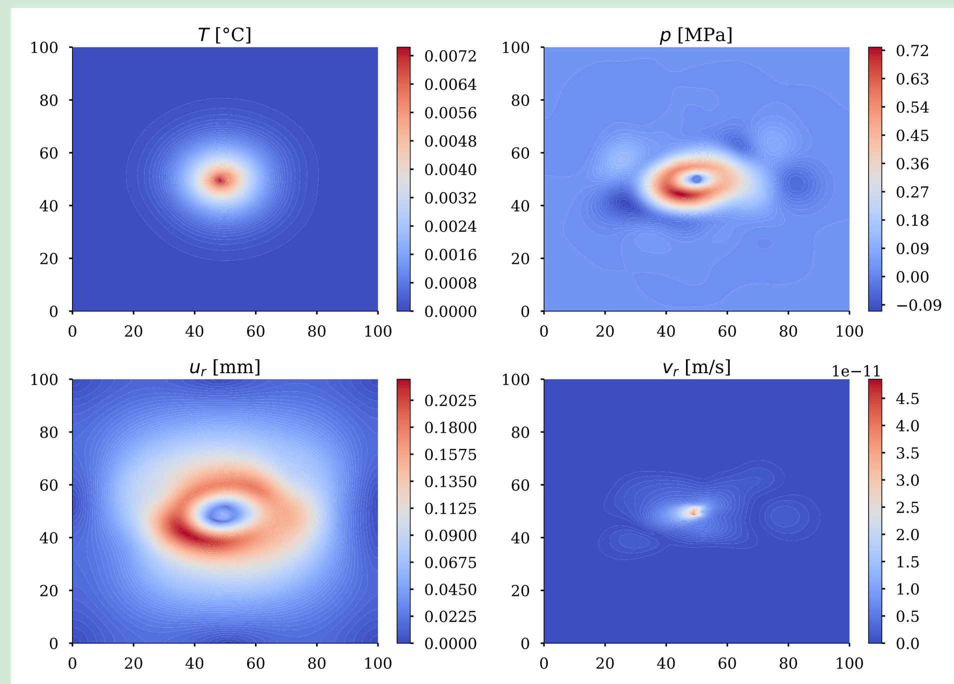
One of the many random realizations



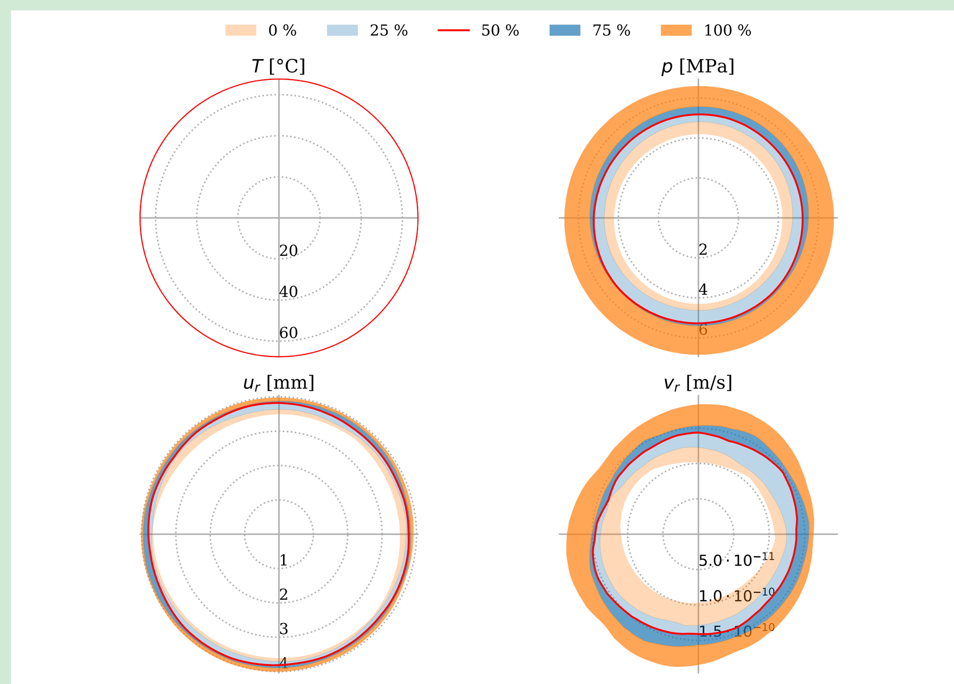
Results: Homogeneous, anisotropic



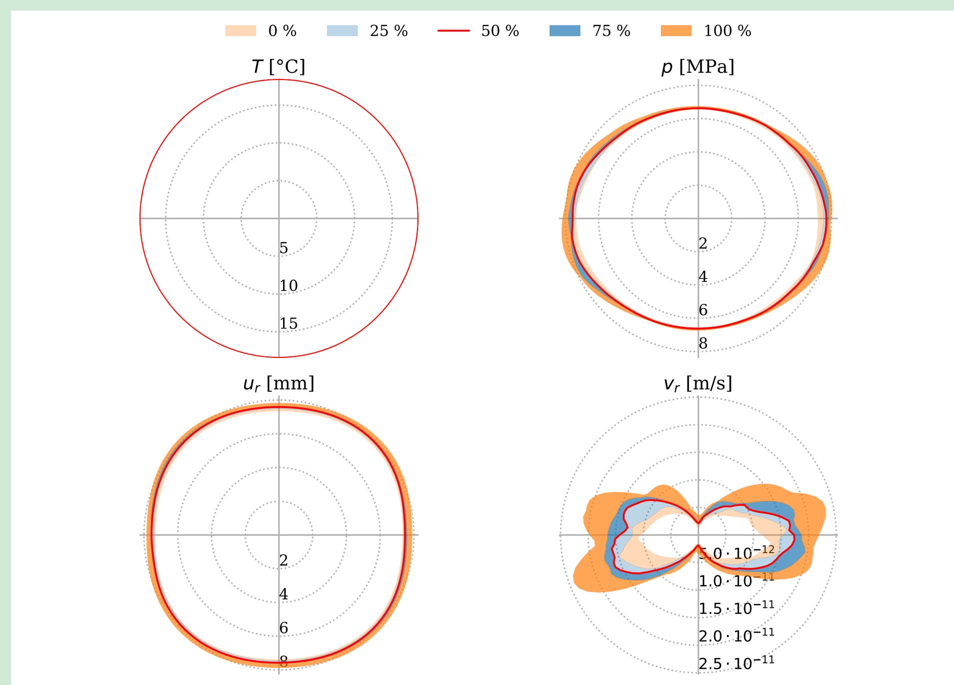
Results: Heterogeneous, hydraulically anisotropic (Mean of diff.)



Results: Heterogeneous, isotropic at $r = 5\,\mathrm{m}$



Results: Heterogeneous, hydraulically anisotropic at $r = 25\,\mathrm{m}$



Conclusions / outlook

- Temperature evolution is not affected by heterogeneity or anisotropy in intrinsic permeability. Same as observed by Chaudhry et al. 2021
- Work in progress. (Early to draw concrete conclusions)
- Statistical anisotropy –> Different correlation lengths
- Random anisotropy –> $k_\perp \neq a\,k_\parallel$?
- Extension to analyse at least one parameter for each process; –> Permeability for p (currently used), –> Thermal conductivity for T, –> Young's modulus for u_S
- Different boundary conditions –> Unsaturated settings (complex ?)
- Better ways to interpret results

References:

[1] Aqeel Afzal Chaudhry, Jörg Buchwald, and Thomas Nagel. "Local and global spatio-temporal sensitivity analysis of thermal consolidation around a point heat source". In: *International Journal of Rock Mechanics and Mining Sciences* 139 (2021), p. 104662. ISSN: 1365-1609.

[2] Herwig R Müller, Benoit Garitte, Tobias Vogt, Sven Köhler, Toshihiro Sakaki, Hanspeter Weber, Thomas Spillmann, Marian Hertrich, Jens K Becker, Niels Giroud, et al. "Implementation of the full-scale emplacement (FE) experiment at the Mont Terri rock laboratory". In: *Mont Terri Rock Laboratory, 20 Years: Two Decades of Research and Experimentation on Claystones for Geological Disposal of Radioactive Waste* (2018), pp. 289–308.

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