Effects of Inhomogeneity and (Statistical and Material) Anisotropy on THM simulations

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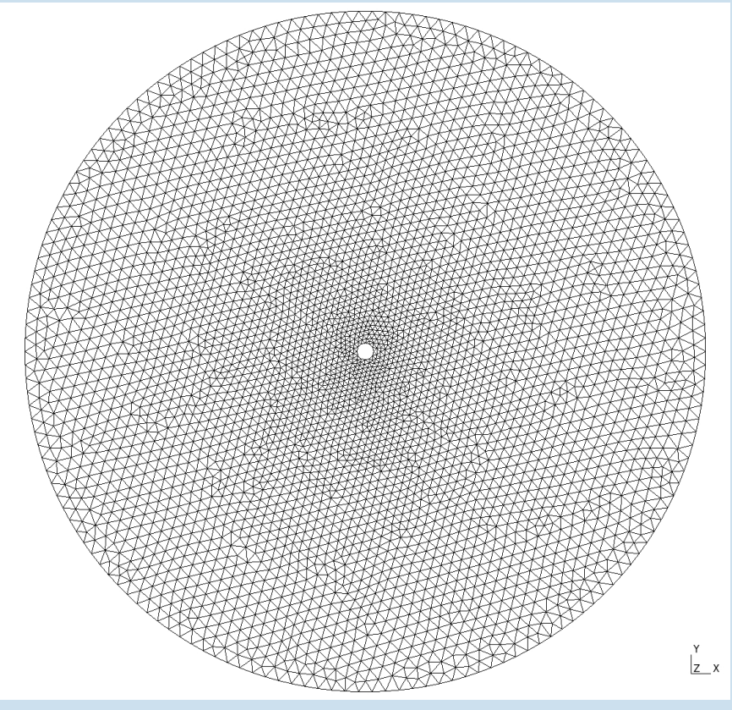
Motivation and highlights

- Investigations into the integrity of barriers [Kurgyis et al. 2024]
- Coupled numerical THM simulations with OpenGeoSys-6 [Bilke et al. 2022]
- Consideration of the uncertainty of input parameters
- Effects of the transverse isotropy of the input parameters
- Input parameters as inhomogeneous random fields
- Consideration of statistical and material anisotropy

Model setup and specifics



- Simplified 2D mesh based on the FE experiment [Müller et al. 2018]
- Host rock (Opalinus Clay) → $d = 100\,\mathrm{m}$
- Circular heat source with a diameter of $2.48\,\mathrm{m}$ → emplaced waste cell
- Thermal conductivity ($\boldsymbol{\lambda}$), intrinsic permeability ($\mathbf{k}$), and elasticity moduli (E_i) as uncertain input parameters
- Generation of inhomogeneous random fields with `kleme`
- Effects on temperature, pore water pressure, displacement, Darcy velocity, von-Mises, and hydrostatic effective stresses.

Initial and boundary conditions:
$T_0 = 15\,°\mathrm{C}$, $p_0 = 2\,\mathrm{MPa}$, $u_{\mathrm{S}0} = 0$

- $\vec{q} \cdot \vec{n}$ at the tunnel boundary
- $p = 0$ at the tunnel boundary
- Normal $\vec{u}_{\mathrm{S}} = \vec{0}$ at the 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

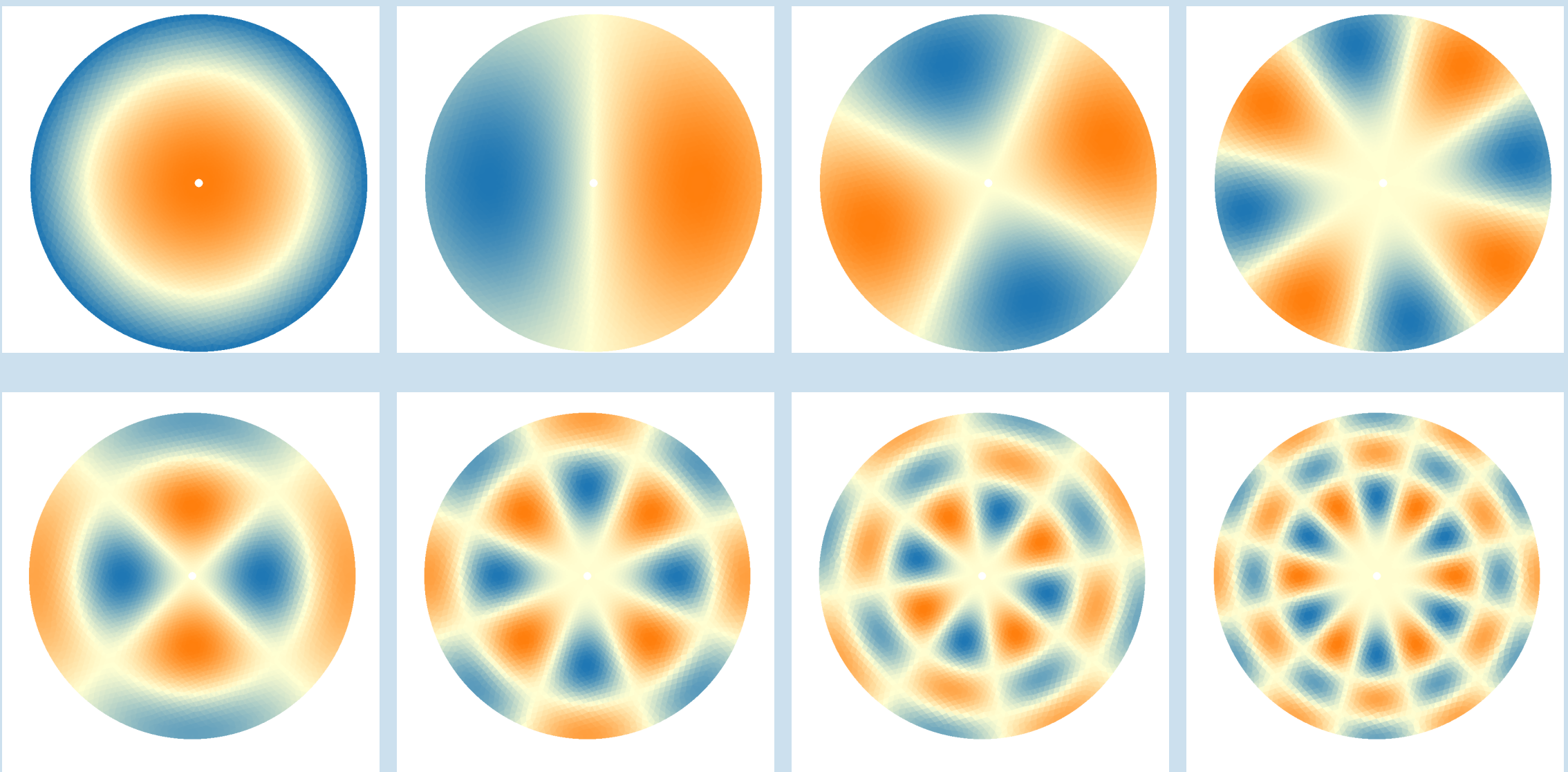
$$(Cu)(\mathbf{x}) = \int_D c(\mathbf{x},\mathbf{y})u(\mathbf{y})\mathrm{d}\mathbf{y}$$

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

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

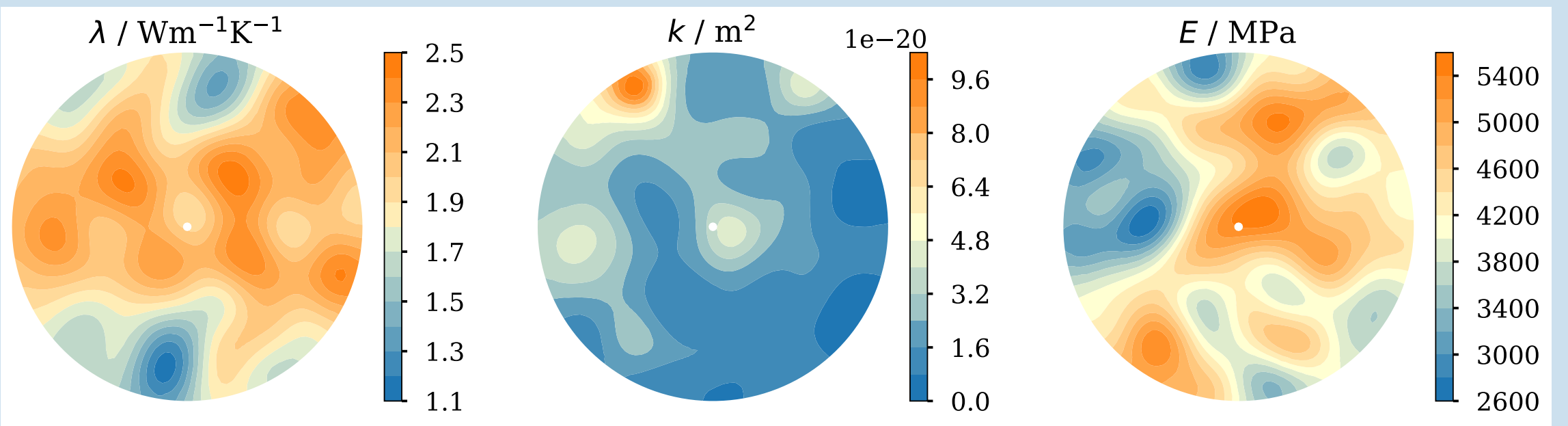
where σ is the scale factor and l is the correlation length.



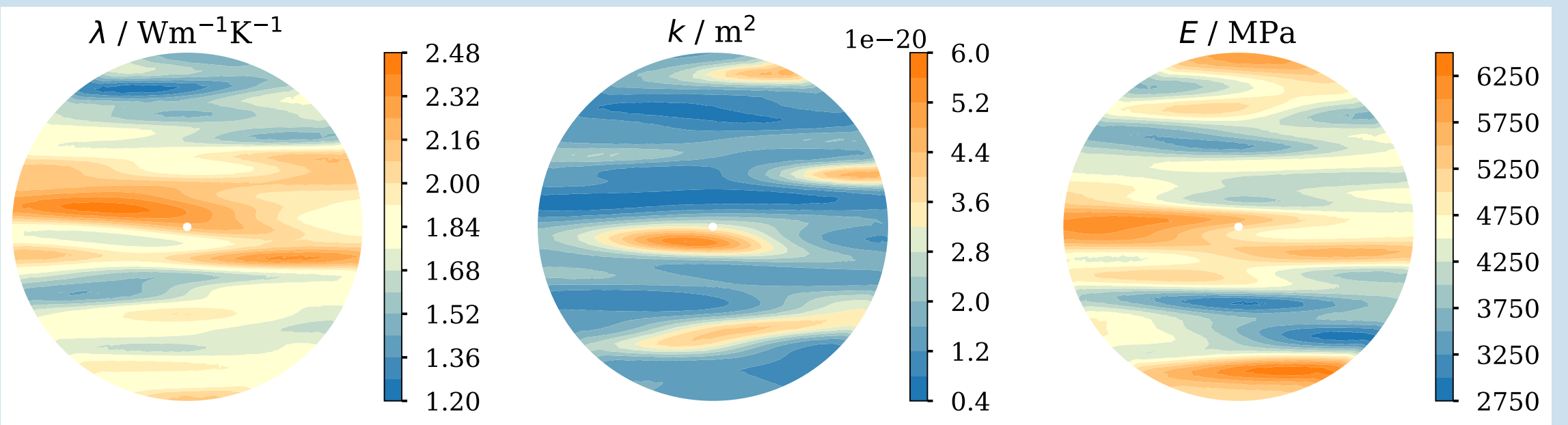
Eigenfunctions 1, 2, 5, 11, 13, 25, 43, and 64 of the domain of interest, using a Matérn covariance function with smoothness parameter $\nu = 0.5$ and characteristic length $\ell = 15\,\mathrm{m}$. The outer diameter of the domain is set to $100\,\mathrm{m}$. Orange hues indicate higher values and a colorbar is omitted as the relative magnitudes of the eigenfunctions are not of primary interest in this context.

Examples of inhomogeneous random fields

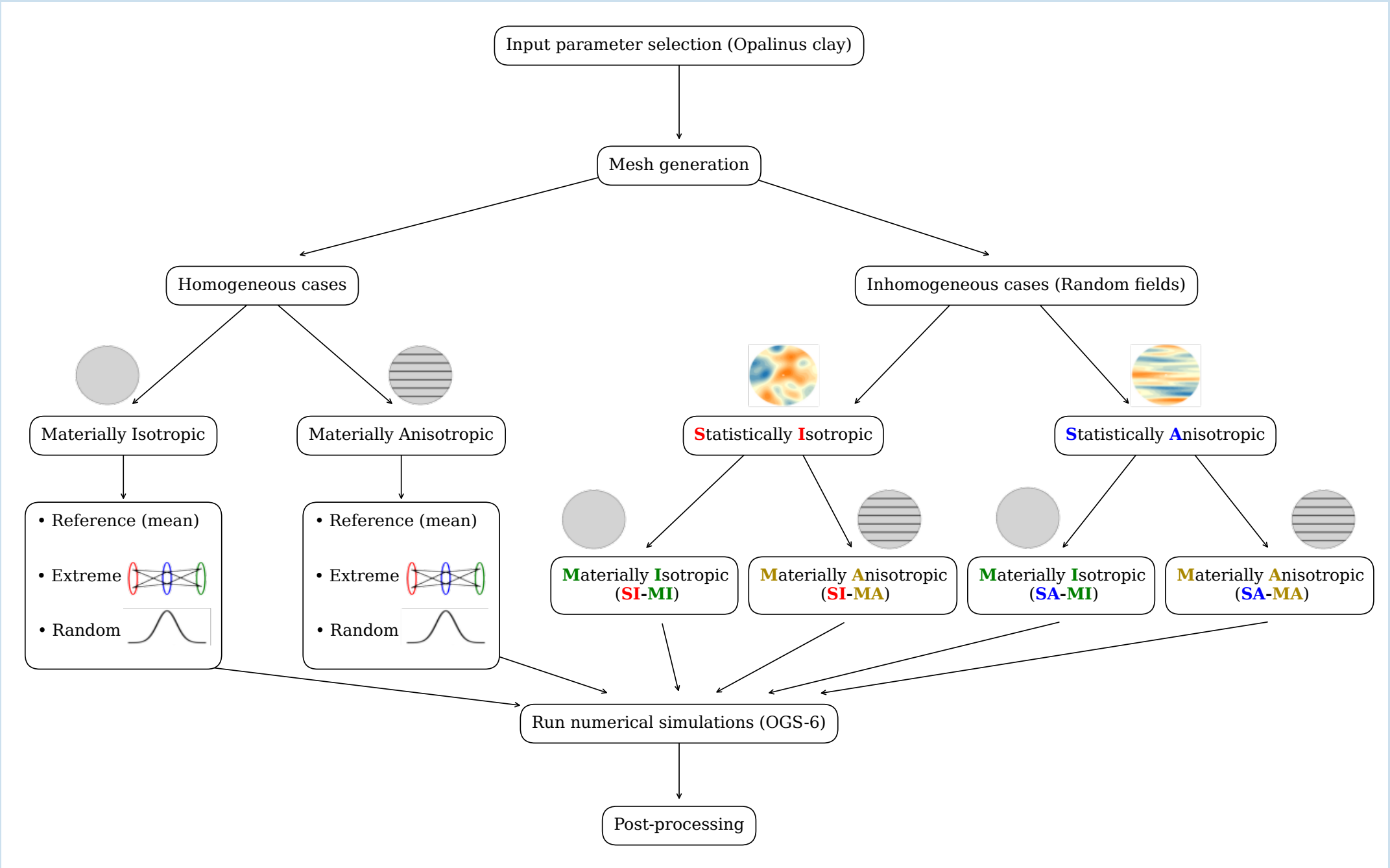
- Statistically Isotropic case



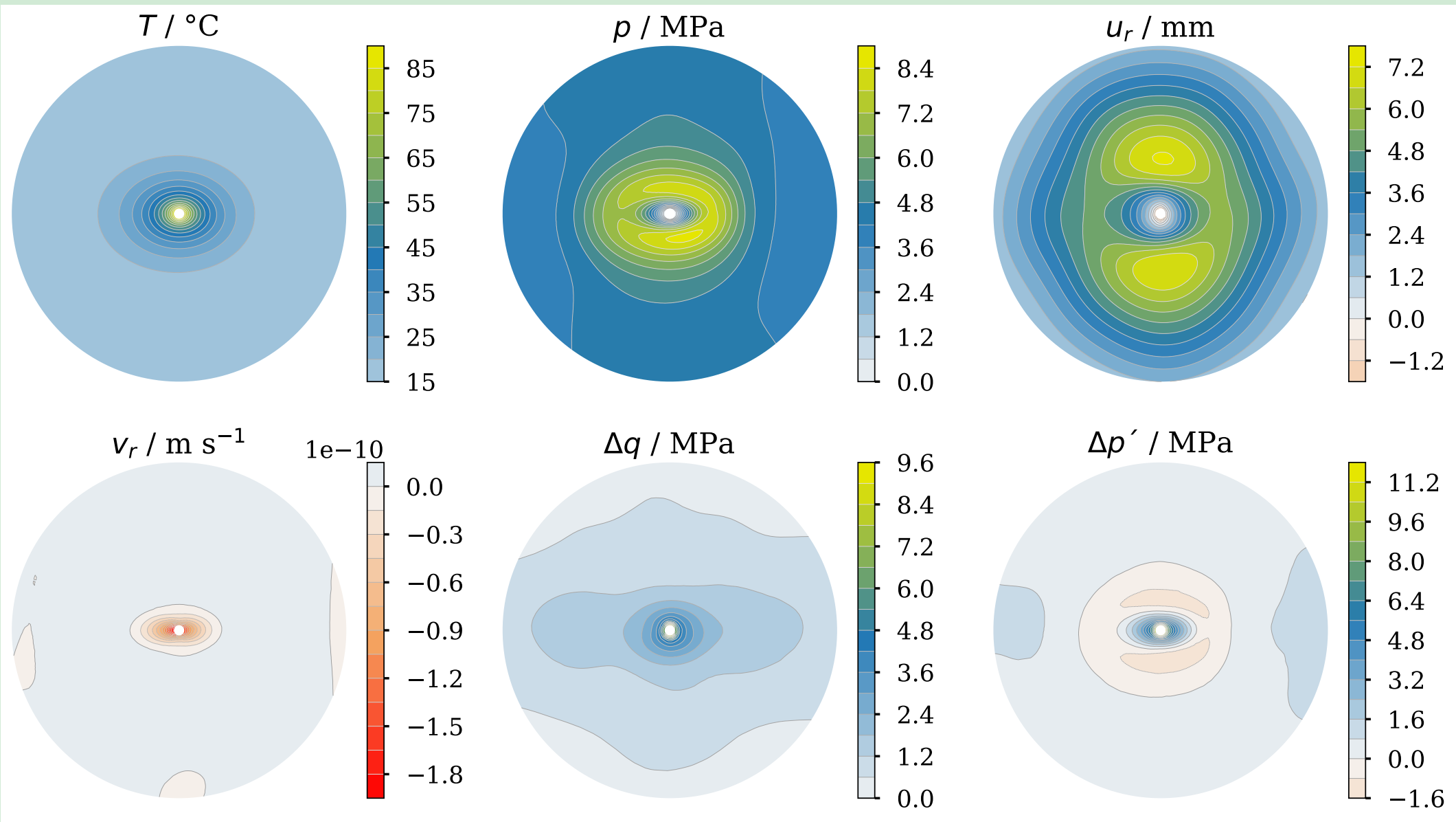
- Statistically Anisotropic case



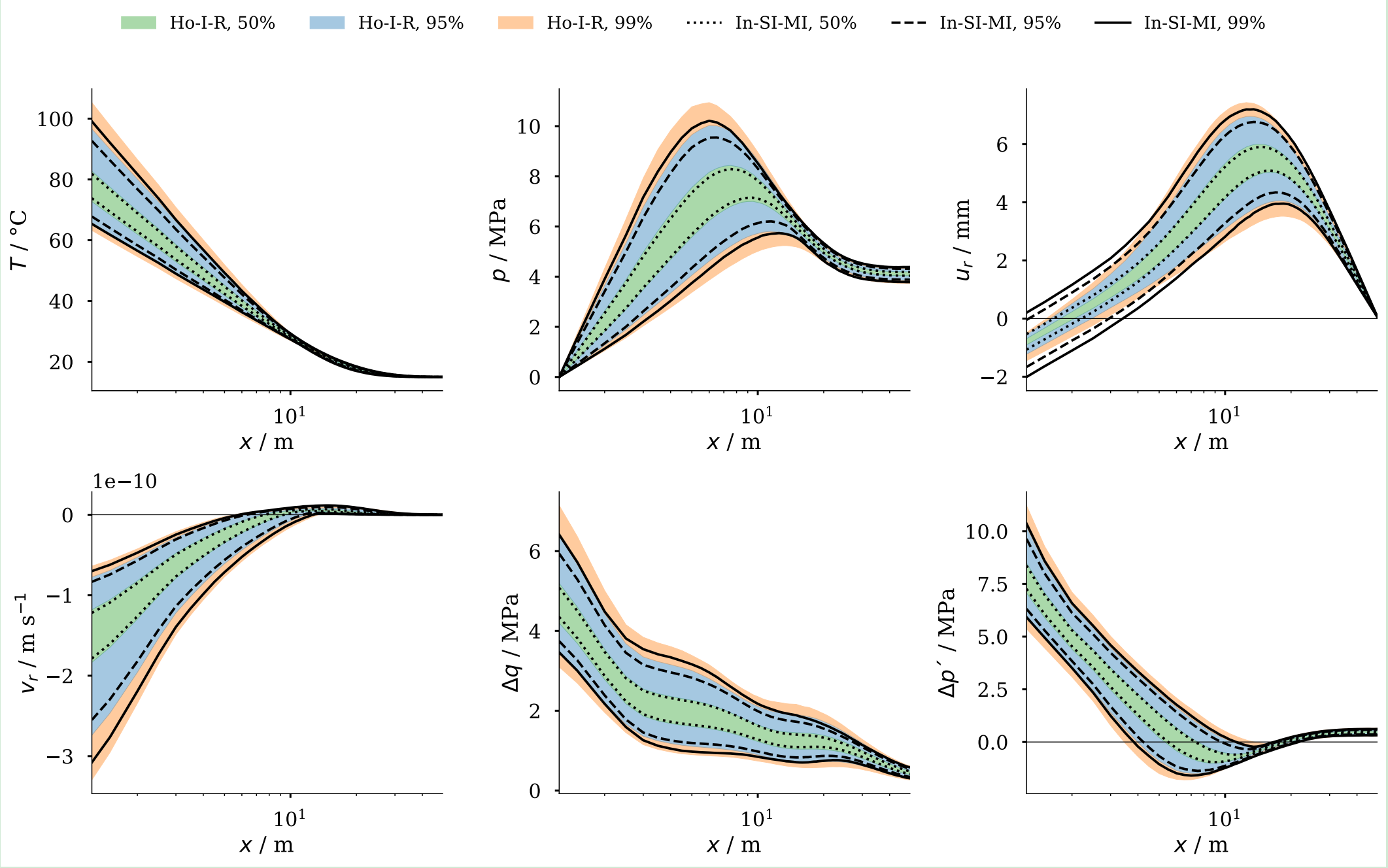
Workflow



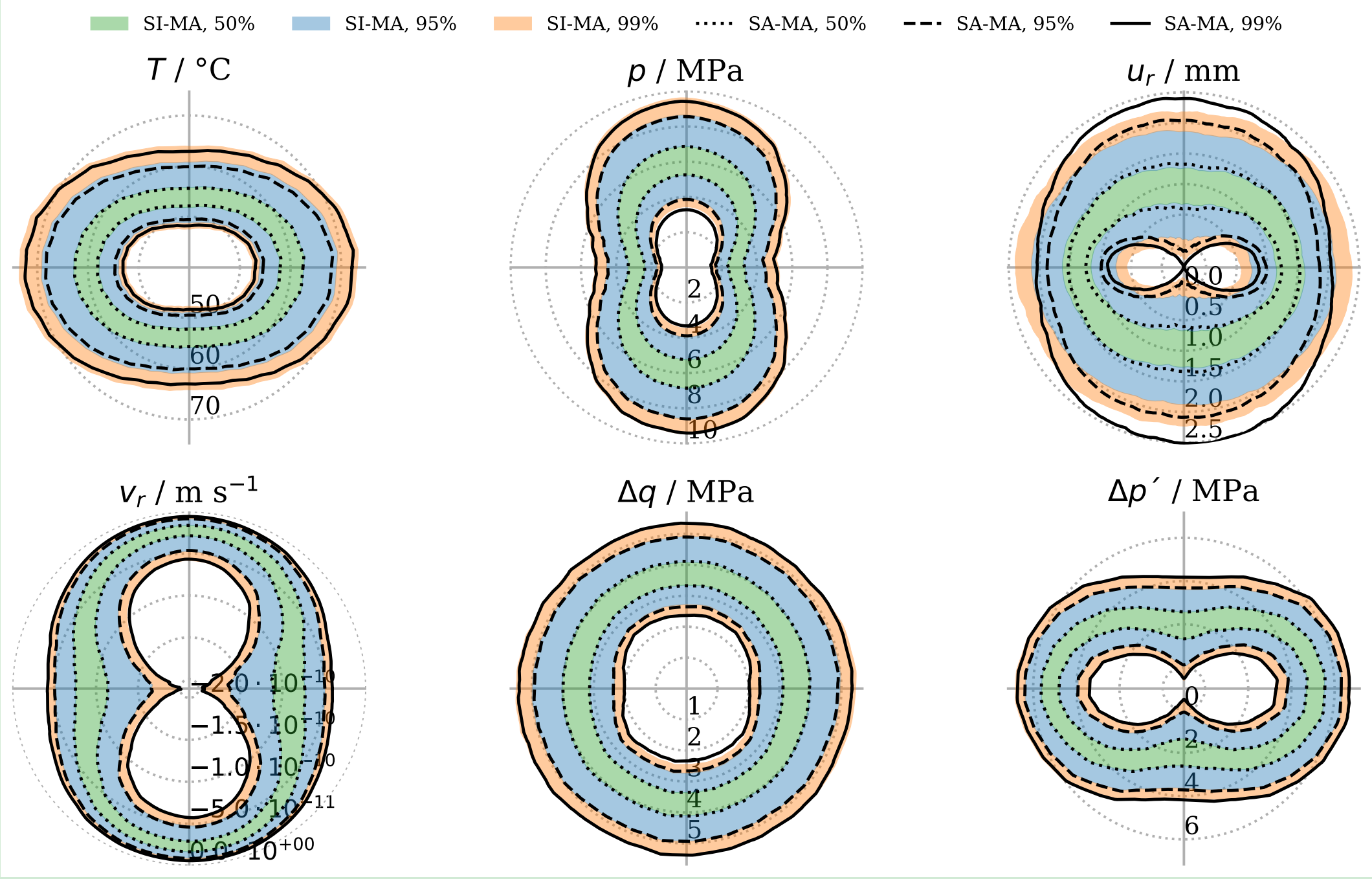
Results



Contour plot for statistically isotropic and materially anisotropic case using one random realization of a random field for input parameters up to a radius of $r = 40\,\mathrm{m}$



Plot showing comparison of various inter-percentile ranges (IPR) of output variables for $10\,000$ realizations of random fields of input parameters along the x-axis for the homogeneous-isotropic (Random) and inhomogeneous-isotropic (SI-MI) case.



Polar plot showing $50\,\%$, $95\,\%$ and $99\,\%$ IPR for the statistically isotropic and anisotropic cases in the presence of material anisotropy for all output variables at a distance of $3\,\mathrm{m}$ from the heat source.

Conclusions

- The temperature development is not influenced by inhomogeneity or anisotropy of the intrinsic permeability and stiffness; see also Chaudhry et al. 2021.
- The effect of statistical anisotropy is visible even in the absence of material anisotropy.
- Stress-based indicators show that material anisotropy has a more pronounced effect than statistical anisotropy.
- Interpretation of results with regard to integrity criteria.

Outlook

- Introduce varying statistical anisotropy ratios (instead of fully correlated fields).
- Include additional uncertain parameters (e.g., bentonite layers).
- Validate and calibrate models using field-scale data.
- Investigate surrogate modeling to reduce computational costs.

References:

[1] Lars Bilke, Christoph Lehmann, Dmitry Naumov, Thomas Fischer, Wenqing Wang, Jörg Buchwald, Karsten Rink, Norbert Grunwald, Florian Zill, Feliks K Kiszkurno, et al. "OpenGeoSys". In: *Zenodo* (2022).

[2] 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.

[3] Kata Kurgyis, Peter Achtziger-Zupančič, Merle Bjorge, Marc S Boxberg, Matteo Broggi, Jörg Buchwald, Oliver G Ernst, Judith Flügge, Andrey Ganopolski, Thomas Graf, et al. "Uncertainties and robustness with regard to the safety of a repository for high-level radioactive waste: introduction of a research initiative". In: *Environmental Earth Sciences* 83.2 (2024), p. 82.

[4] 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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