Inhomogeneity and anisotropy in THM-coupled integrity calculations

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FLASHBACK – EXPECTED PLAN FOR MEQUR

Starting point –> FE experiment
Planned study steps

- Selection of input parameters for SA/UQ
  –> based on knowledge from previous studies like Buchwald et al. 2020; Chaudhry et al. 2021
- Survey of available data sources (BGR)
  –> parameter inhomogeneities, (auto)correlation lengths
- Simplified 2D circular mesh/model based on FE experiment
- Use of as realistic data as possible from the original FE experiment
- Initial study based on 1 parameter (hydraulic conductivity <–> intrinsic permeability)
- Extension to other parameters like E, λ, α_s, c_p, ϕ

What's new?

- Added a study case for extreme values
- Added a study case for homogeneous random values
- Added two cases for statistical anisotropy
- Removal of bugs in the code, improved color-maps

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Governing equations – TRM (Pitz et al. 2023)

Heat balance:

$$\begin{aligned}(\rho c_p)_{\mathsf{eff}} \frac{\mathrm{d}T}{\mathrm{d}t} + L_0 \frac{\mathrm{d}\theta_{\mathsf{vap}}}{\mathrm{d}t} - \operatorname{div}\left(\boldsymbol{\lambda}_{\mathsf{eff}} \operatorname{grad} T\right)\\ + \operatorname{div}\left(\frac{L_0 \boldsymbol{J}_{\mathsf{G}}^{\mathsf{W}}}{\rho_{\mathsf{GR}}^{\mathsf{W}}}\right) + \operatorname{grad} T \cdot \left(c_{p\mathsf{L}} \boldsymbol{A}_{\mathsf{L}} + c_{p,\mathsf{vap}} \boldsymbol{J}_{\mathsf{G}}^{\mathsf{W}}\right) = Q_T\end{aligned}$$

Mass balance:

$$\begin{aligned}&\rho_{\mathsf{LR}} S_{\mathsf{L}} (\alpha_{\mathsf{B}} - \phi) \beta_{p,\mathsf{SR}} \frac{\mathrm{d}p_{\mathsf{LR}}}{\mathrm{d}t} - \rho_{\mathsf{LR}} S_{\mathsf{L}} (\alpha_{\mathsf{B}} - \phi) \operatorname{tr}(\boldsymbol{\alpha}_{T,\mathsf{SR}}) \frac{\mathrm{d}T}{\mathrm{d}t}\\ &+ \phi \left((1 - S_{\mathsf{L}}) \frac{\mathrm{d}\rho_{\mathsf{GR}}^{\mathsf{W}}}{\mathrm{d}t} + S_{\mathsf{L}} \frac{\mathrm{d}\rho_{\mathsf{LR}}}{\mathrm{d}t} \right) + (\rho_{\mathsf{LR}} - \rho_{\mathsf{GR}}^{\mathsf{W}}) \left[\phi + p_{\mathsf{LR}} S_{\mathsf{L}} (\alpha_{\mathsf{B}} - \phi)\right] \frac{\mathrm{d}S_{\mathsf{L}}}{\mathrm{d}t}\\ &+ \rho_{\mathsf{LR}} S_{\mathsf{L}} \alpha_{\mathsf{B}} \operatorname{div}\left(\frac{\mathrm{d}\boldsymbol{u}_{\mathsf{S}}}{\mathrm{d}t}\right) + \operatorname{div}\left(\boldsymbol{A}_{\mathsf{L}}^{\mathsf{W}} + \boldsymbol{J}_{\mathsf{G}}^{\mathsf{W}}\right) = Q_H\end{aligned}$$

Momentum balance:

$$\operatorname{div}\left(\boldsymbol{\sigma}^{\mathsf{eff}} - \alpha_{\mathsf{B}} \chi(S_{\mathsf{L}}) p_{\mathsf{LR}} \mathbf{I}\right) + \rho \mathbf{g} = \mathbf{0}$$

with

$$\dot{\boldsymbol{\sigma}}^{\mathsf{eff}} = \boldsymbol{\mathcal{C}} : (\dot{\boldsymbol{\epsilon}} - \dot{\boldsymbol{\epsilon}}_{\mathsf{pl}} - \dot{\boldsymbol{\epsilon}}_{\mathsf{th}} - \dot{\boldsymbol{\epsilon}}_{\mathsf{sw}})$$

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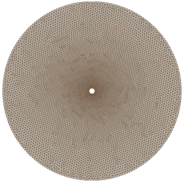
Model setup and specifics

- Simplified 2D mesh: $d = 100\,\mathrm{m}$
  –> host rock (Opalinus clay)
- Circular heat source of $d = 2.48\,\mathrm{m}$
  –> emplaced waste cell
- Aninsotropic –> Transverse isotropy
  –> parallel and perpendicular to bedding plane
- Inhomogeneous input parameters
  –> Random Inhomogeneous Field Generator Code
  –> TU Chemnitz
- Uncertainty quantification using numerical modeling
  –> TRM –> OpenGeoSys
- Comparison of results with homogeneous, isotropic models



Simplified 2D mesh

Initial conditions:
$T_0 = 15\,^\circ\mathrm{C}$, $p_0 = 2\,\mathrm{MPa}$, $u_{\mathrm{S}0} = 0$

Boundary conditions:

- Q_T (Neumann) at tunnel boundary
- $p = 0$ at tunnel boundary
- $u_{\mathrm{S}} = 0$ on outer boundary

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Tab. 1: Input parameters.

Parameter	Symbol / Unit	Low	Best	High	Distribution
Thermal conductivity (isotropic)	λ_{iso} / $\mathrm{W\,m^{-1}\,K^{-1}}$	1.31	1.85	2.39	Normal
Thermal conductivity (parallel)	$\lambda_{\parallel}$ / $\mathrm{W\,m^{-1}\,K^{-1}}$	1.7	2.4	3.1	Normal
Thermal conductivity (normal)	$\lambda_{\perp}$ / $\mathrm{W\,m^{-1}\,K^{-1}}$	0.92	1.3	1.68	Normal
Intrinsic permeability (isotropic)	k_{iso} / $\mathrm{m^2}$	$0.6 \cdot 10^{-20}$	$2.25 \cdot 10^{-20}$	$6 \cdot 10^{-20}$	Log-normal
Intrinsic permeability (parallel)	$k_{\parallel}$ / $\mathrm{m^2}$	$1 \cdot 10^{-20}$	$3.75 \cdot 10^{-20}$	$10 \cdot 10^{-20}$	Log-normal
Intrinsic permeability (normal)	$k_{\perp}$ / $\mathrm{m^2}$	$0.2 \cdot 10^{-20}$	$0.75 \cdot 10^{-20}$	$2 \cdot 10^{-20}$	Log-normal
Young's modulus (isotropic)	E_{iso} / MPa	3000	4500	6000	Normal
Young's modulus (parallel)	$E_{\parallel}$ / MPa	4000	6000	8000	Normal
Young's modulus (normal)	$E_{\perp}$ / MPa	2000	3000	4000	Normal

STUDY CASES

–> Let f be the parameter in question (f in this study –> λ, k, E)

Homogeneous cases:

- Isotropic –> $f_x = f_y = \text{mean}(f_{\text{iso}})$
- Anisotropic –> $f_x = \text{mean}(f_{||}), \quad f_y = \text{mean}(f_{\perp})$
- Isotropic –> $f_x = f_y$
  –> Extremes: combinations of min, max of f_{iso}, sims $= 2^3 = 8$
  –> Random: Random values of f_{iso}, sims $=10000$
- Ansotropic –> $f_x \neq f_y$
  –> Extremes: combinations of min, max of $f_{||}$ and $f_{\perp}$ respectively, sims $= 2^3 = 8$
  –> Random: Random values of $f_{||}$ and $f_{\perp}$ respectively, sims $=10000$

Inhomogeneous cases:

- statistically isotropic, materially isotropic
  –> CL$_x$ = CL$_y$ $= 15\,\text{m}$, –> f_{iso}(RF)
- statistically isotropic, materially anisotropic
  –> CL$_x$ = CL$_y$ $= 15\,\text{m}$, –> $f_{||}$(RF), $f_{\perp}$(RF)
- statistically anisotropic, materially isotropic
  –> CL$_x$ $= 50\,\text{m}$, CL$_y$ $= 5\,\text{m}$, –> f_{iso}(RF)
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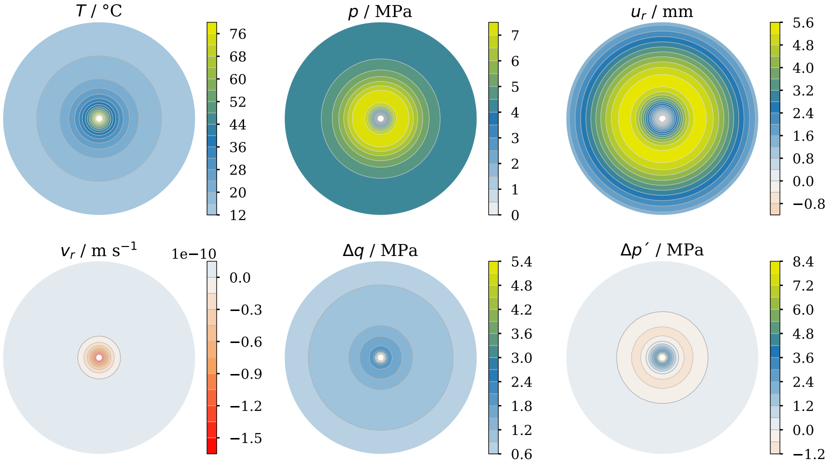
–> $\Delta q = \sqrt{\frac{3}{2}\sigma'_{\mathrm{d}} : \sigma'_{\mathrm{d}}}$ $\quad \Delta p' = -\frac{1}{3}\sigma'_{ii}$

Homogeneous, isotropic (reference) case



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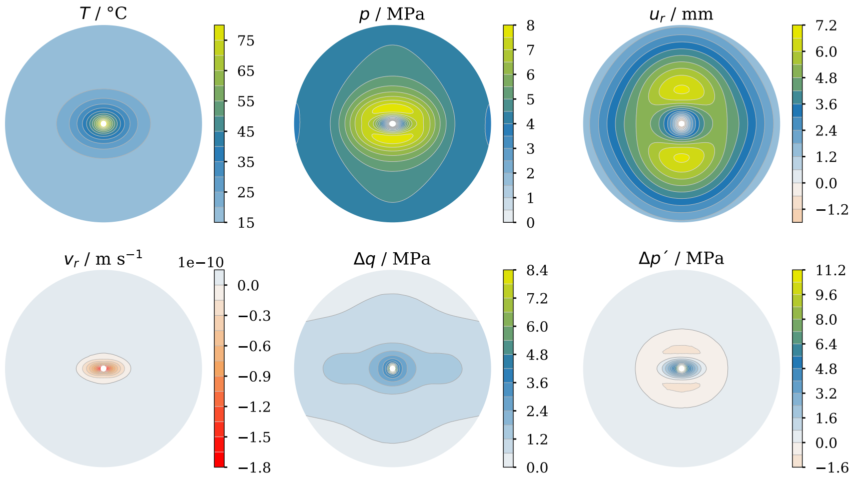
Homogeneous, anisotropic case



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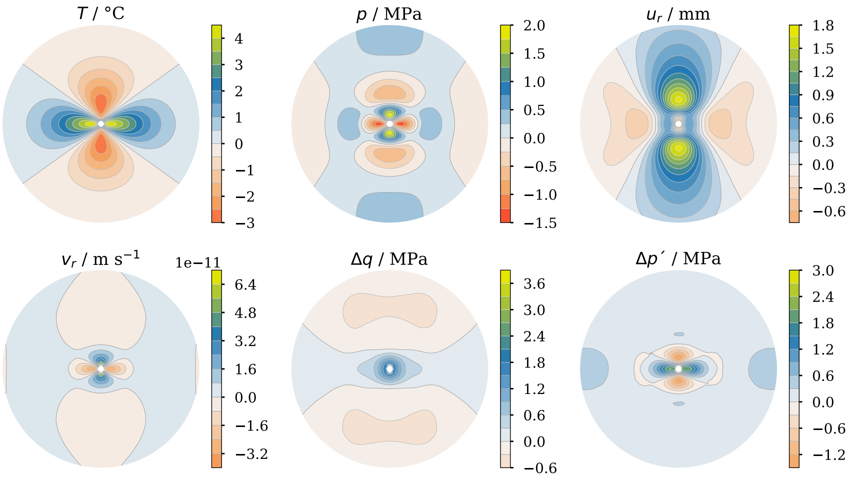
Diff. between iso and anisotropic



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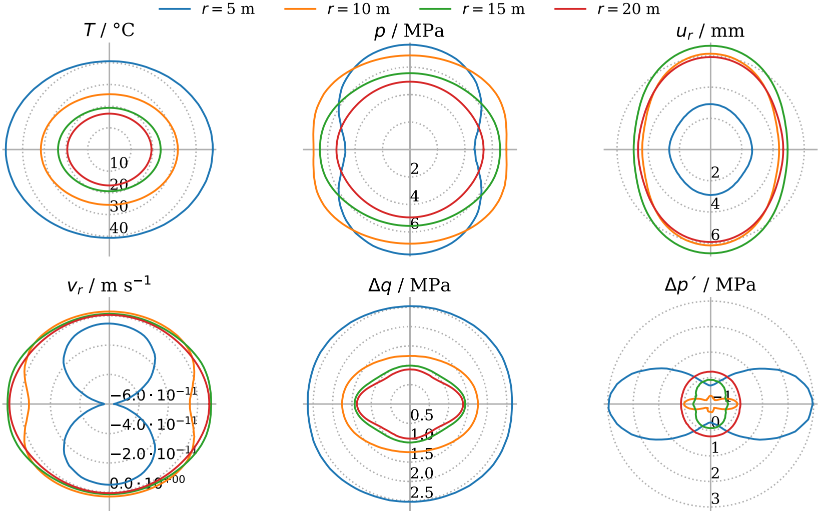
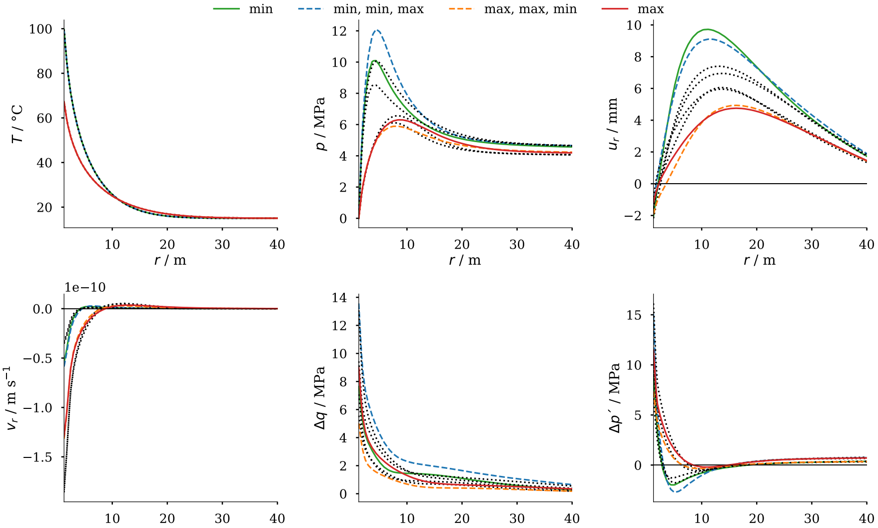
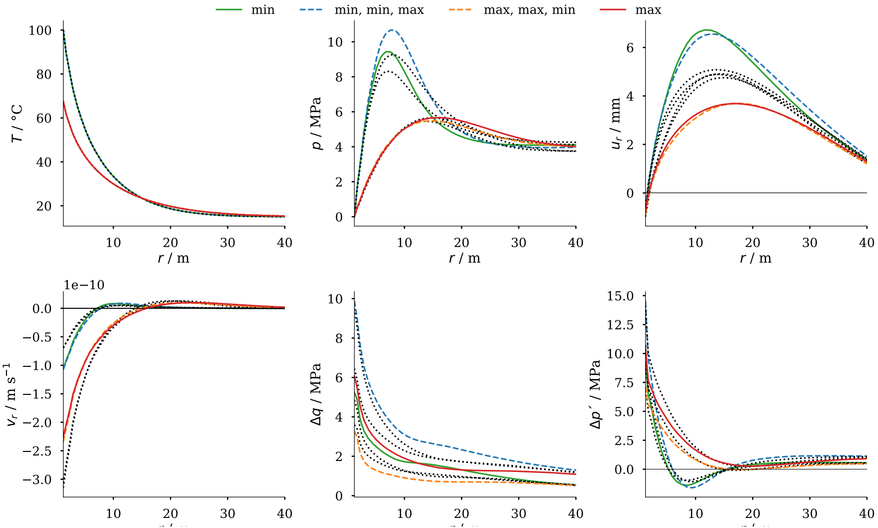
Homogeneous, anisotropic case



Homogeneous, anisotropic case (extremes) (along y-axis)



Homogeneous, anisotropic case (extremes) (along x-axis)



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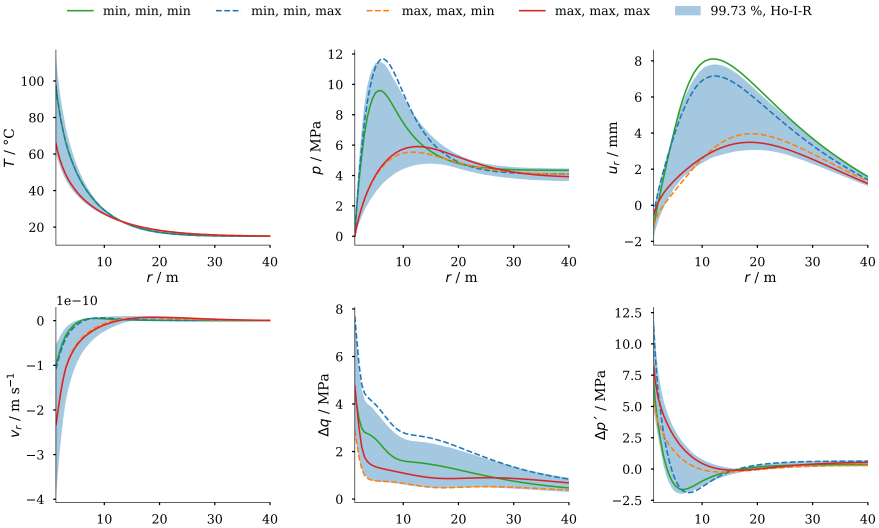
Homogeneous, isotropic case (extremes vs random)



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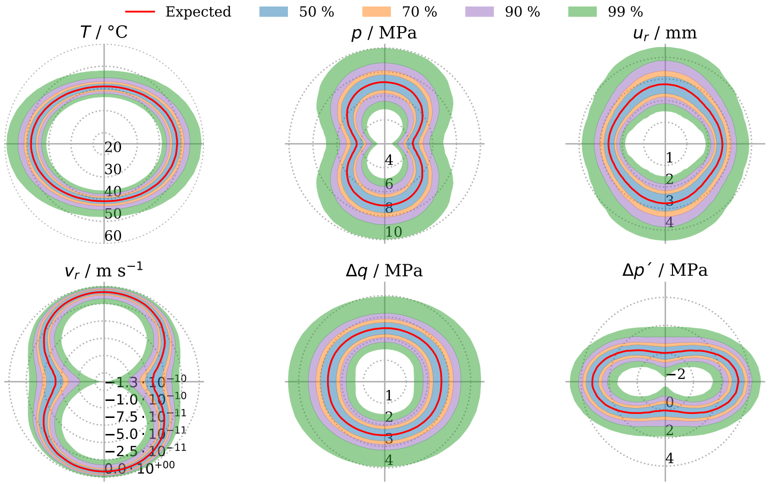
Homogeneous, anisotropic case (random) $r = 5\,\mathrm{m}$



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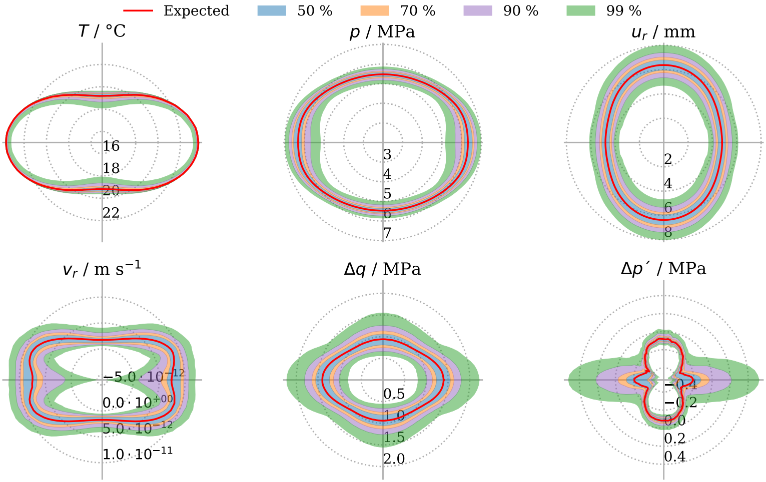
Homogeneous, anisotropic case (random) $r = 15\,\mathrm{m}$



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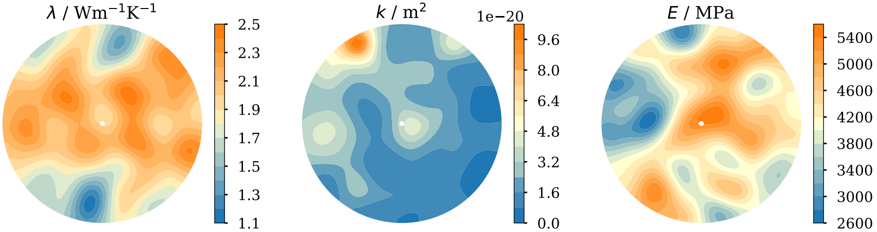
Inhomogeneity and anisotropy in THM-coupled integrity calculations

- Example of one random realisation (stat. isotropy)



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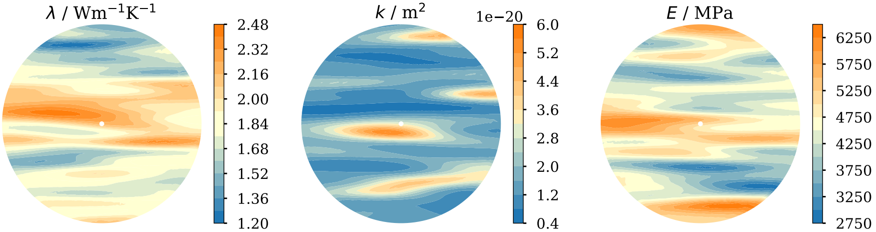

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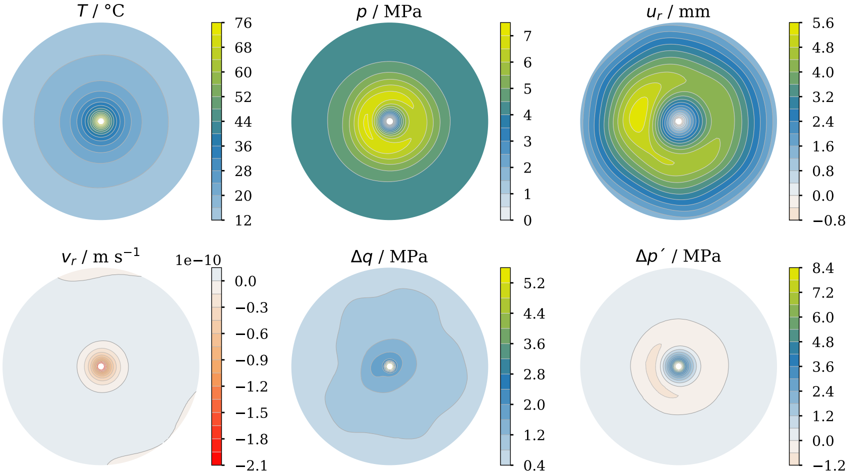
Stat. isotropic, mat. isotropic case (one realization)



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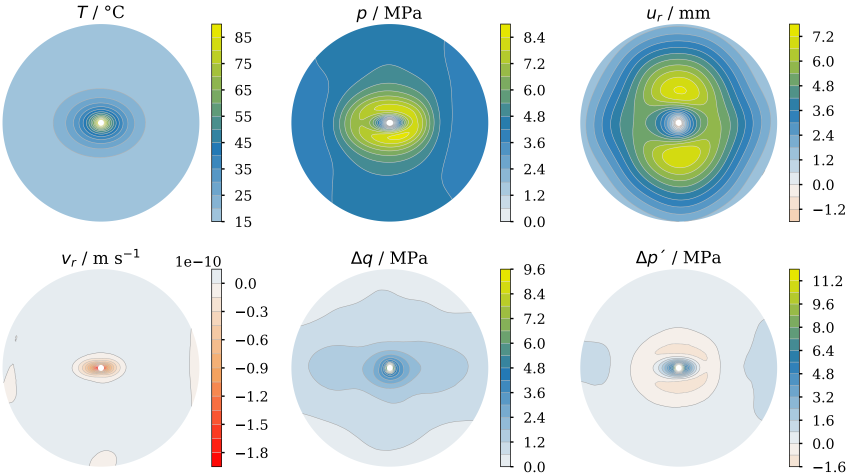

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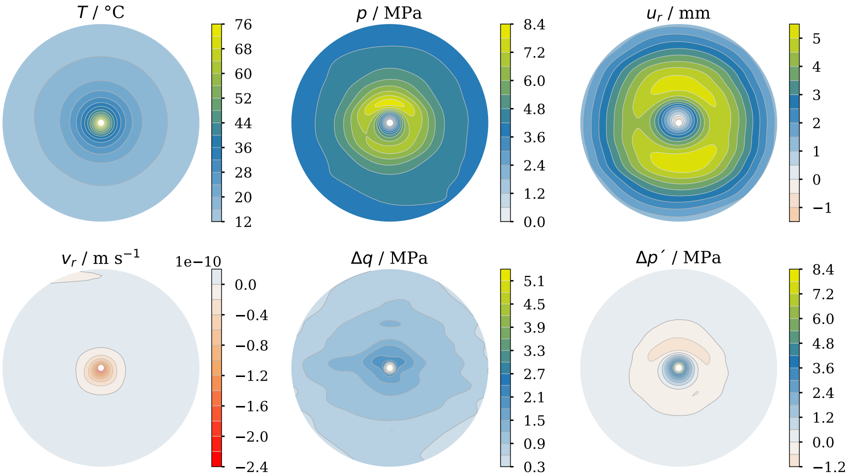

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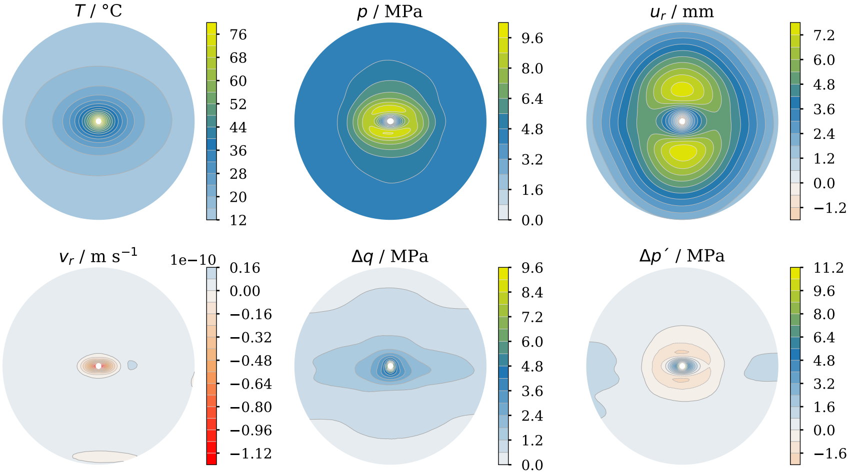
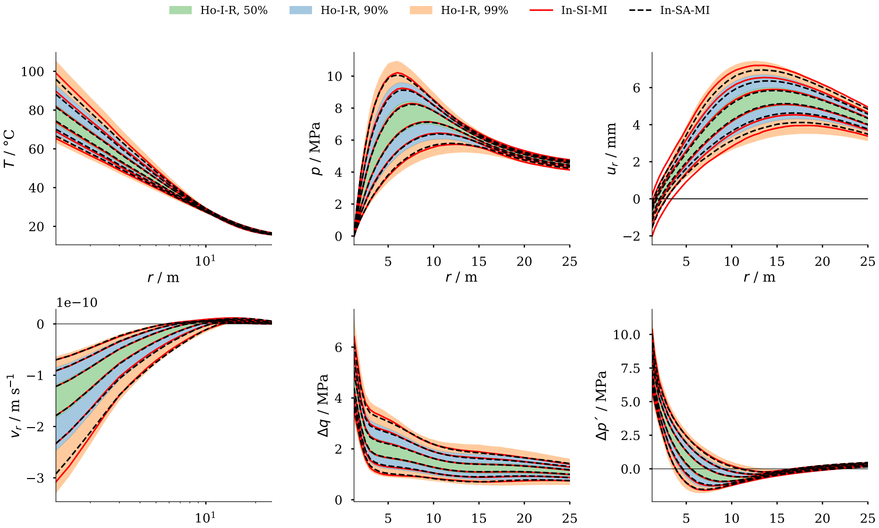


Comparison between all materially isotropic cases



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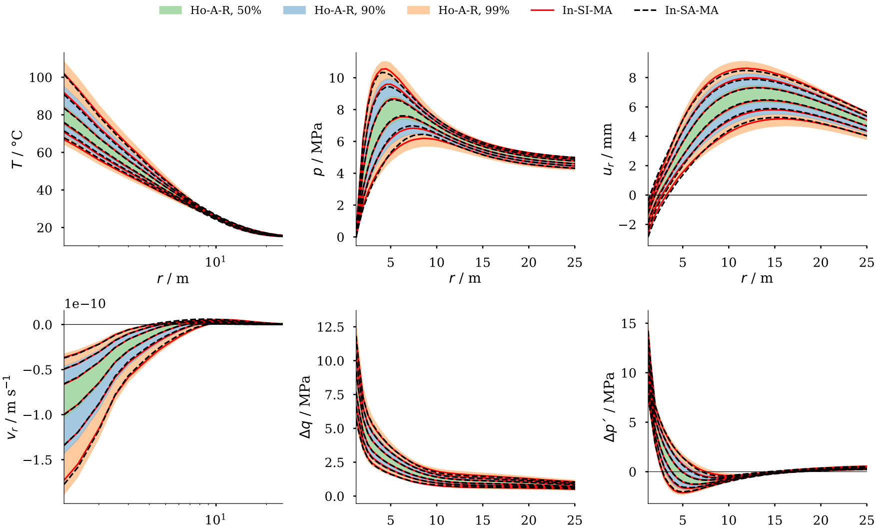

Summary and outlook

- 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 also visible in the absence of material anisotropy
- Using extreme or random homogenous values may result in overly strict integrity criteria
- Interpretation in relation to integrity criteria
- Random anisotropy
  –> $f_\perp \neq a_f \, f_{||}$?
- Different boundary conditions (?)
- Unsaturated settings (?) (complex)

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BGE BUNDESGESELLSCHAFT FÜR ENDLAGERUNG

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