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UNIVERSITY OF TECHNOLOGY IN THE EUROPEAN CAPITAL OF CULTURE CHEMNITZ

Uncertainties in THM-coupled integrity calculations

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Visit:

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https://tu-freiberg.de/bodenmechanik

https://www.tu-chemnitz.de/mathematik/numa/

URS PhDs Workshop | Kassel | Germany | 16-17 Mar., 2023

OUTLINE

Parameter uncertainity in THM process – Feliks

Inhomogeneity and anisotropy in THM simulations – Aqeel

`kleme`: C++ library for generating random fields – Chao (Charlie)

INTRODUCTION - UNCERTAINITY & THERMO OSMOSIS

Uncertainities

- Parameter uncertainity
- Measurement uncertainity
- Inhomogenity of clay
- Model uncertainity

Thermo osmosis (TO)

- Fluid flow driven by a temperature gradient
- Unit: $\mathrm{Pa} * \mathrm{m} * \mathrm{K}^{-1}$

INTRODUCTION - ATLAS EXPERIMENT

Geometry of experiment

- 2D, axisymmetric
- 100m x 119m
- Observation point at: $(1.515, 14.0)$

Numerical setup

- Processes:
  - Thermo Hydro Mechanical (THM)
  - Thermo Hydro Mechanical with thermo osmosis (THM+TO)
- Isotropy is assumed

Goals

- Match pressure and temperature observations
- Test if TO improves match between observed data and simulation

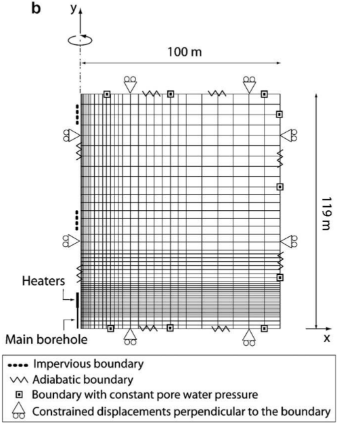


Fig. 1: Layout of ATLAS Experiment. Figure from: François et al. 2009

AHM - MESH CONVERGENCE STUDY

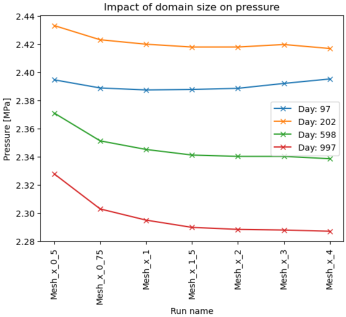


Fig. 2: Convergence of pressure depending on the size of the simulation domain.

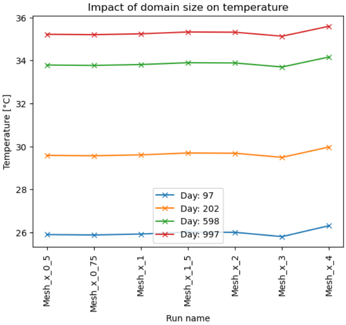


Fig. 3: Convergence of temperature depending on the size of the simulation domain.

AHM - OVERVIEW

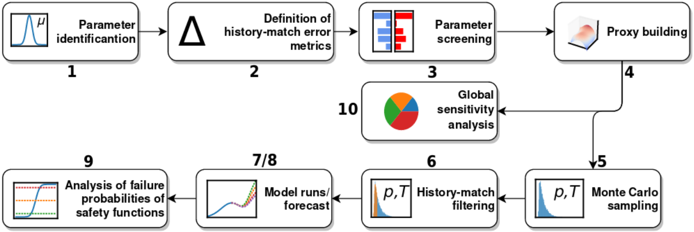


Fig. 4: History matching and uncertainty quantification workflow, Figure from Buchwald et al. 2020

AHM - PARAMETER IDENTIFICATION & ERROR METRICS

Tested parameter ranges

Parameter name	Unit	Reference	Min	Max
Thermal expansivity (α_s)	K^{-1}	$1.3e-5$	$1.3e-6$	$1.3e4$
Intrinsic permeability (k)	m^2	$2.5e-19$	$4e-20$	$7e-19$
Thermoosmosis coefficient (k_T)	$\mathrm{Pa}*\mathrm{m}*\mathrm{K}^{-1}$	$5e-11$	$1e-13$	$1e-10$
Young's modulus (E)	MPa	$3.5e8$	$2e8$	$4e8$
Poissons ratio (ν)	-	0.125	0.1	0.2

Error metrics

$$e_{HM} = \sum_{1}^{n} \frac{(d_{obs} - d_{sim})^2}{n} \tag{1}$$

alternatively:

$$e_{HM} = max(abs(d_{obs} - d_{sim})) \tag{2}$$

AHM - PARAMETER SCREENING - OVAT - PRESSURE

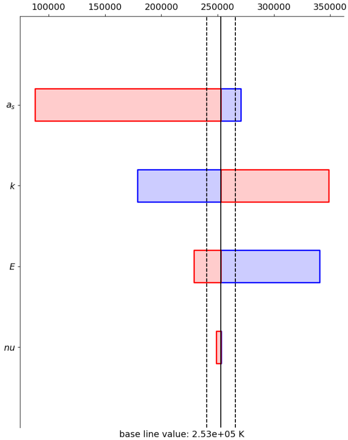


Fig. 5: Results of OVAT test for pressure with **THM** process. Dashed line indicate threshold of statistical significance. Unit: Pa.

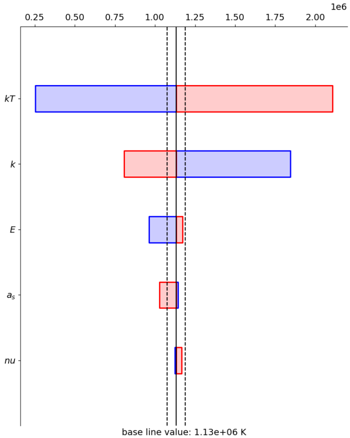


Fig. 6: Results of OVAT test for pressure with **THM+TO** process. Dashed line indicate threshold of statistical significance. Unit: Pa.

AHM - PROXY

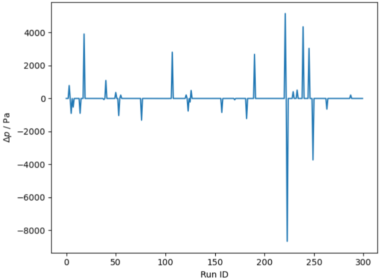


Fig. 7: Overview of proxy error for history matching error for pressure. Trained on 270 out 300 runs with 30 used for evaluation.

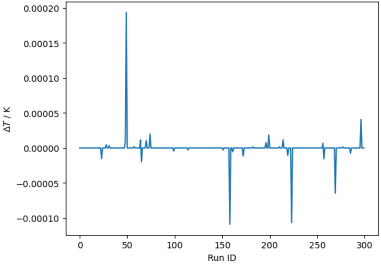


Fig. 8: Overview of proxy error for history matching error for temperature. Trained on 270 out 300 runs with 30 used for evaluation.

AHM - HM - RESULTS - BEST PARAMETERS VALUES

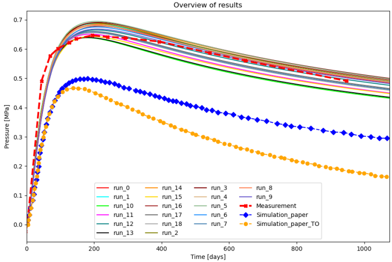


Fig. 9: Overview of simulation results of 19 best results obtained from Monte-Carlo sampling (**THM** process)

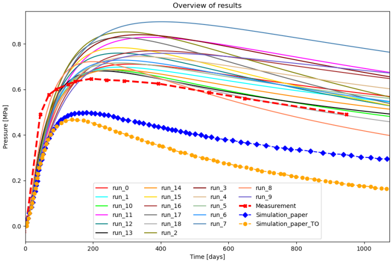


Fig. 10: Overview of simulation results of 19 best results obtained from Monte-Carlo sampling (**THM+TO** process)

AHM - HM - RESULTS - THM+TO

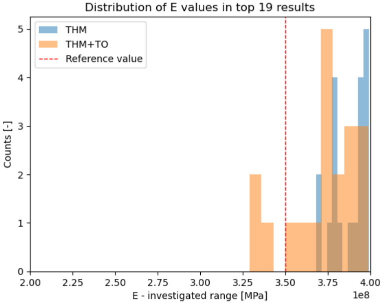


Fig. 11: Histogramm comparing distribution of 19 values of E from 19 best simulation results for **THM** and **THM+TO** processes.

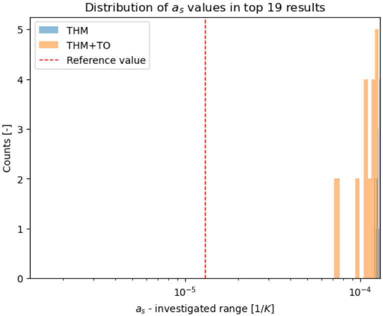


Fig. 12: Histogramm comparing distribution of 19 values of a_s from 19 best simulation results for **THM** and **THM+TO** processes.

AHM - HM - BEST PARAMETERS VALUES

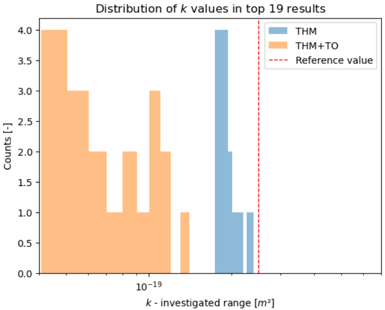


Fig. 13: Histogramm comparing distribution of 19 values of k from 19 best simulation results for **THM** and **THM+TO** processes.

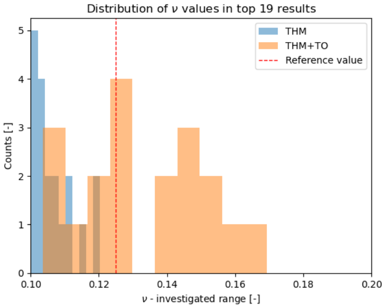


Fig. 14: Histogramm comparing distribution of 19 values of ν from 19 best simulation results for **THM** and **THM+TO** processes.

AHM - PROBLEMS

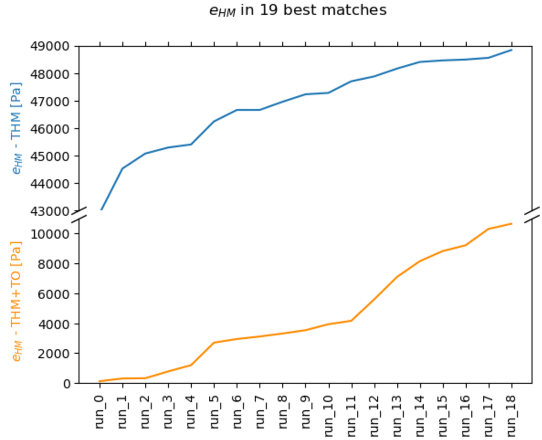


Fig. 15: History matching errors in THM and THM+TO processes.

AHM - PROBLEMS

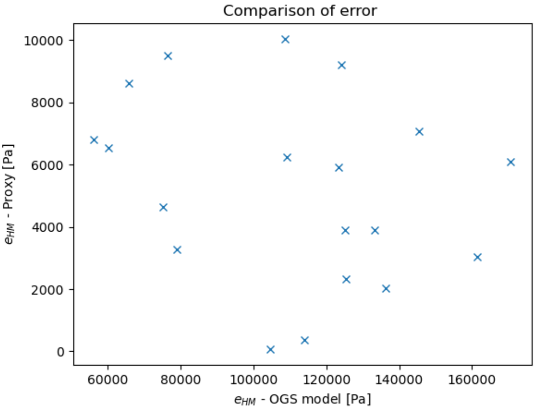


Fig. 16: Comparison of history matching error between proxy and simulation.

AHM - PROBLEMS

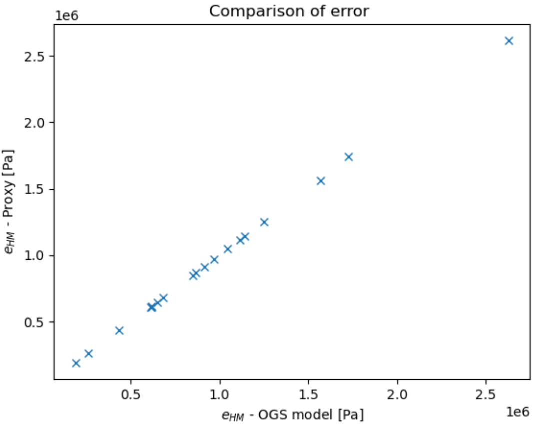


Fig. 17: Comparison of history matching error between proxy and simulation.

AHM - SUMMARY & CONCLUSIONS & NEXT STEPS

Conclusions

- Adding TO has an impact on pressure
- THM+TO changes the preferred values of parameters
- Analysis of proxy errors show that the coverage of certain areas of parameter space may not be sufficient

Next steps

- Veryfing if the impact of TO is due to its physical importance, statistical error or adding additional arbitrary fitting parameter
- Better setup for proxy
- Investigation of metrics
- More rigorous statistical post processing and analysis of results
- Better parametrization of TO
- Finer selection of parameter space

Tossing the ball to Aqeel ;)

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 heterogeneities, (auto)correlation lengths
- Simplified 2D 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)
- Extension to other parameters like E, λ, α_s, c_p, ϕ

Governing equations – TRM

Heat balance:

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

Mass balance:

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

Momentum balance:

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

with

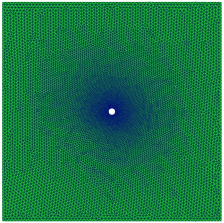
$$\dot{\boldsymbol{\sigma}}^{\text{eff}} = \boldsymbol{\mathcal{C}} : (\dot{\boldsymbol{\epsilon}} - \dot{\boldsymbol{\epsilon}}_{\text{pl}} - \dot{\boldsymbol{\epsilon}}_{\text{th}} - \dot{\boldsymbol{\epsilon}}_{\text{sw}})$$

Inhomogeneity and anisotropy in THM simulations – Aqeel

Model setup and specifics

- Simplified 2D mesh: $100\,\mathrm{m} \times 100\,\mathrm{m}$
  –> host rock (Opalinus clay)
- Circular heat source of $3\,\mathrm{m}$ diameter
  –> emplaced waste cell
- Aninsotropic –> Transverse isotropy
  –> parallel and perpendicular to bedding plane
- Heterogeneous input parameters
  –> Random Heterogeneous Field Generator Code
  –> TU Chemnitz
- Uncertainty quantification using numerical modeling
  –> TRM –> OpenGeoSys
- Comparison of results with homogeneous, isotropic models

Simplified 2D mesh



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

Boundary conditions:

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

CASE STUDIES

–> $k_{||} = 5 \times 10^{-20}\,\mathrm{m}^2$
–> $k_{\perp} = a\,k_{||}$, with $a = 0.2$

- Homogeneous, isotropic
  –> $k_x = k_y = k_{||}$
- Homogeneous, anisotropic
  –> $k_x = k_{||}, \quad k_y = k_{\perp}$
- Heterogeneous, statistically isotropic, hydraulically isotropic
  –> $k_x(\mathrm{RF}) = k_y(\mathrm{RF}) = k_{||}$
- Heterogeneous, statistically isotropic, hydraulically anisotropic
  –> $k_x(\mathrm{RF}) = k_{||}, \quad k_y(\mathrm{RF}) = k_{\perp}$

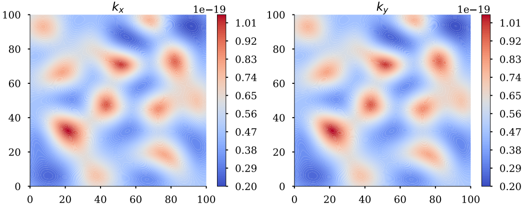
Will not be shown today

- Heterogeneous, statistically anisotropic, hydraulically isotropic
  –> $k_x(\mathrm{RF}_x) = k_{||}, \quad k_y(\mathrm{RF}_y) = k_{||}$
- Heterogeneous, statistically anisotropic, hydraulically anisotropic
  –> $k_x(\mathrm{RF}_x) = k_{||}, \quad k_y(\mathrm{RF}_y) = k_{\perp}$

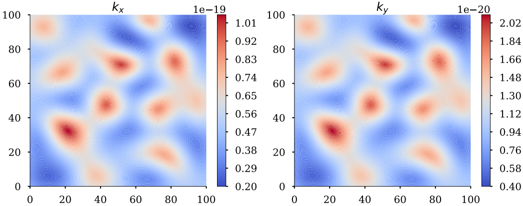
Inhomogeneity and anisotropy in THM simulations – Aqeel

–> Example of one random realisation

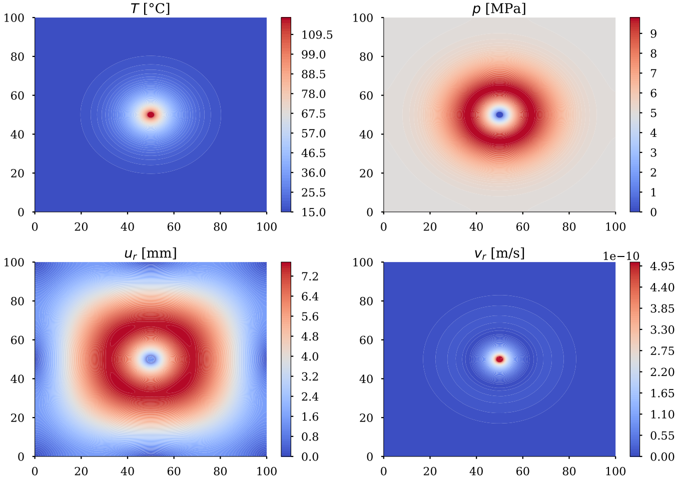
- Heterogeneous, statistically isotropic, hydraulically isotropic



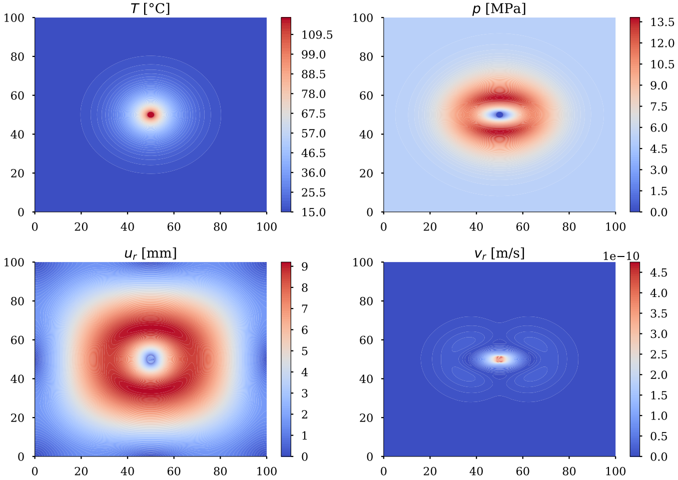
- Heterogeneous, statistically isotropic, hydraulically anisotropic



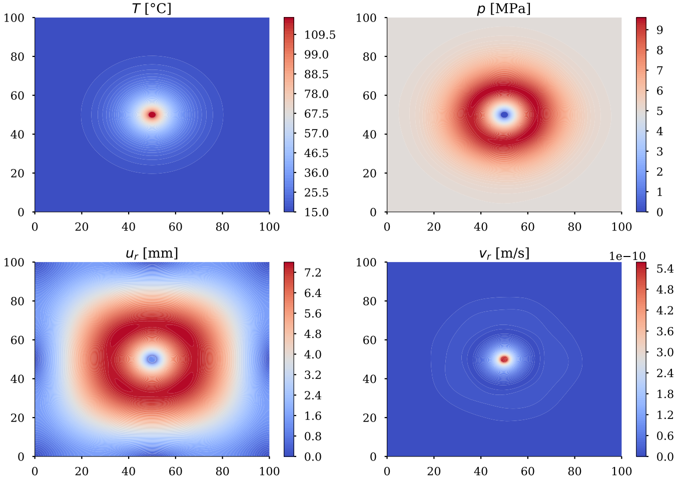
Homogeneous, isotropic (referefence) case



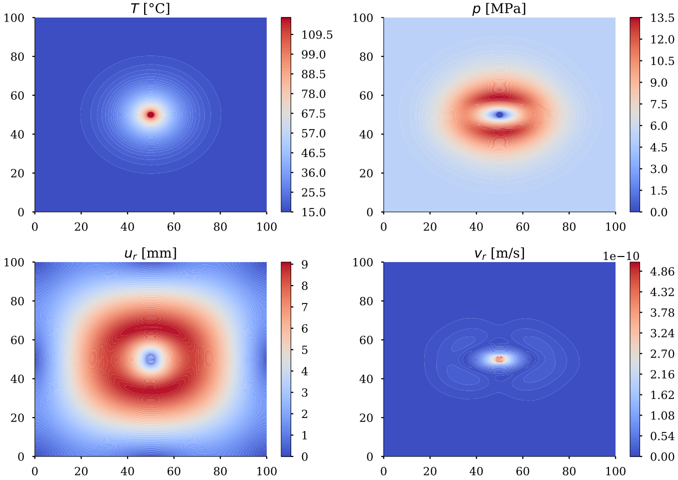
Homogeneous, anisotropic case



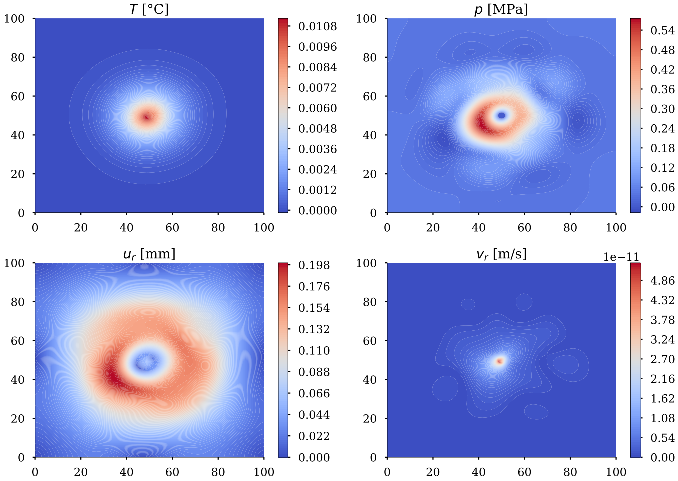
Heterogeneous, statistically isotropic, hydraulically isotropic (Mean)



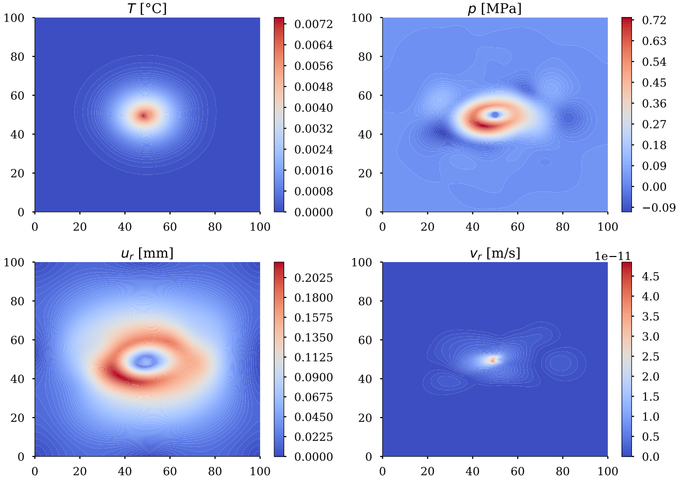
Heterogeneous, statistically isotropic, hydraulically anisotropic (Mean)



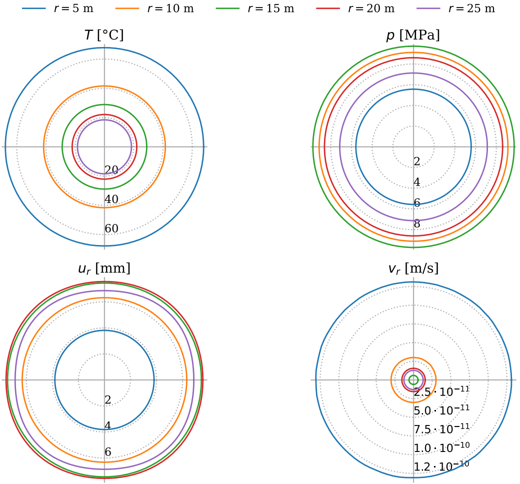
Heterogeneous, statistically isotropic, hydraulically isotropic (Mean of diff.)



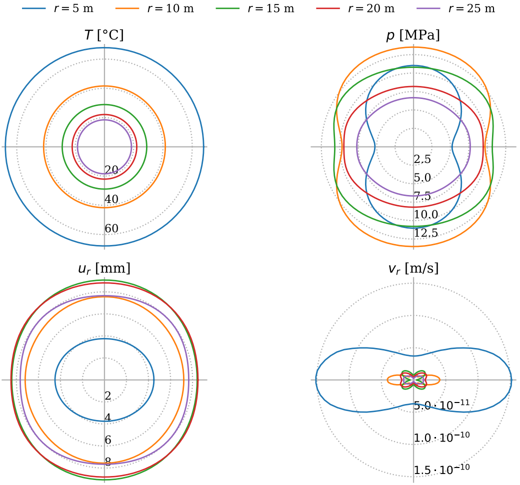
Heterogeneous, statistically isotropic, hydraulically anisotropic (Mean of diff.)



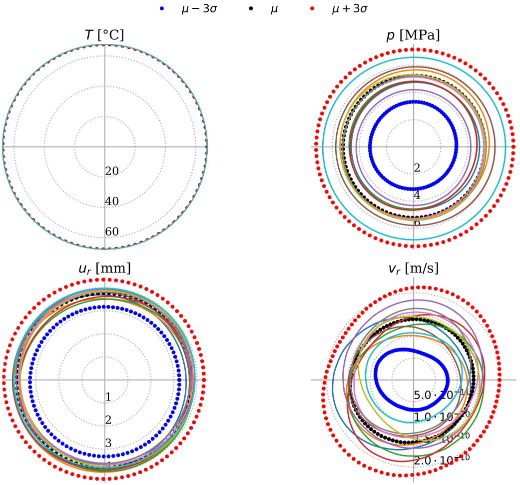
Homogeneous, isotropic (referefence) case



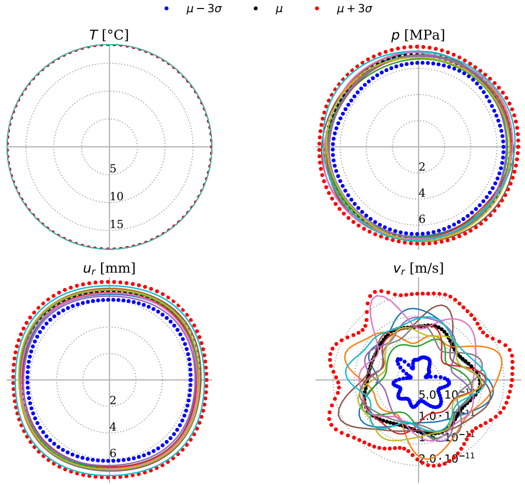
Homogeneous, anisotropic case



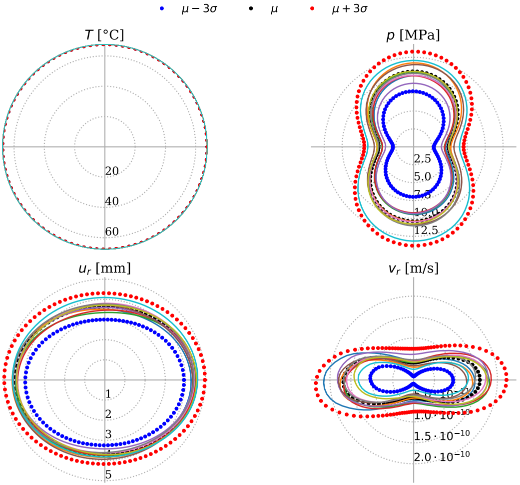
Heterogeneous, statistically isotropic, hydraulically isotropic at $r = 5\,\mathrm{m}$



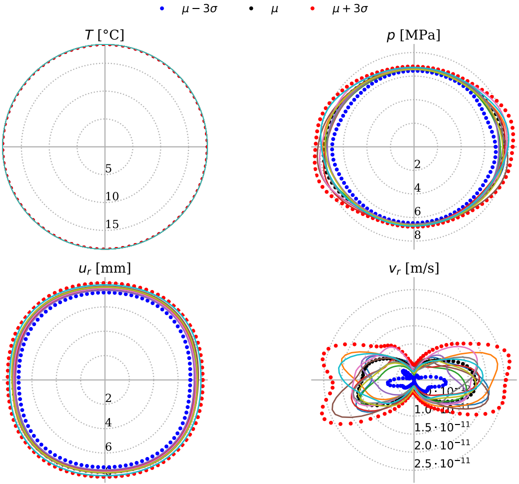
Heterogeneous, statistically isotropic, hydraulically isotropic at $r = 25\,\mathrm{m}$



Heterogeneous, statistically isotropic, hydraulically anisotropic at $r = 5\,\mathrm{m}$



Heterogeneous, statistically isotropic, hydraulically anisotropic at $r = 25\,\mathrm{m}$



Outlook

- 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?

–> Tossing the ball to Charlie!

OUTLINE

`kleme`: a C++ library to efficiently generate random fields for large-scale problems

- review of Karhunen-Loève expansion (KLE)
- numerical difficulties in implementing KLE
- demo code

KARHUNEN-LOÈVE EXPANSION (KLE)

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

λ_i and $\mathbf{f}_i$ are eigenvalues and eigenfunctions, and ξ_i are draws from $\mathcal{N}(0,1)$

KARHUNEN-LOÈVE EXPANSION (KLE)

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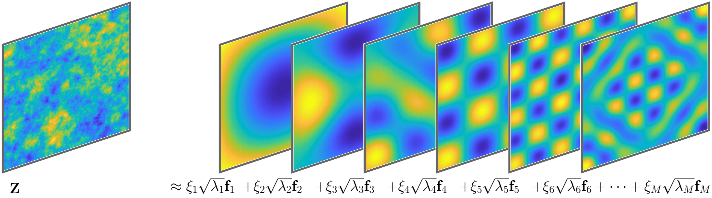

KARHUNEN-LOÈVE EXPANSION (KLE)

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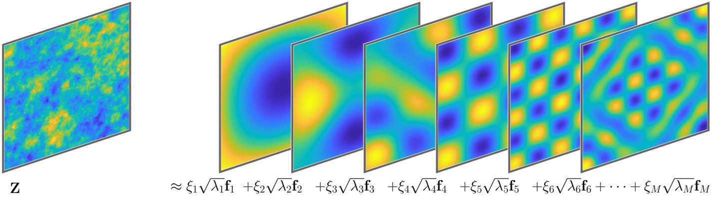


A random field Z represented as a set of $\{\xi_i\}$: dimension reduction

CALCULATION OF λ_I AND F_I

$$\mathbf{C}\mathbf{f}_i = \lambda_i \mathbf{M}\mathbf{f}_i$$

$$[\mathbf{C}]_{i,j} = \int_D \phi_j(\mathbf{x}) \int_D c(\mathbf{x}, \mathbf{y}) \phi_i(\mathbf{y}) \, d\mathbf{y} \, d\mathbf{x}$$

where ϕ is basis function and c is kernel/covariance function

CALCULATION OF λ_I AND F_I

$$\mathbf{C}\mathbf{f}_i = \lambda_i \mathbf{M}\mathbf{f}_i$$

$$[\mathbf{C}]_{i,j} = \int_D \phi_j(\mathbf{x}) \int_D c(\mathbf{x}, \mathbf{y}) \phi_i(\mathbf{y}) \, d\mathbf{y} \, d\mathbf{x}$$

where ϕ is basis function and c is kernel/covariance function

Difficulties

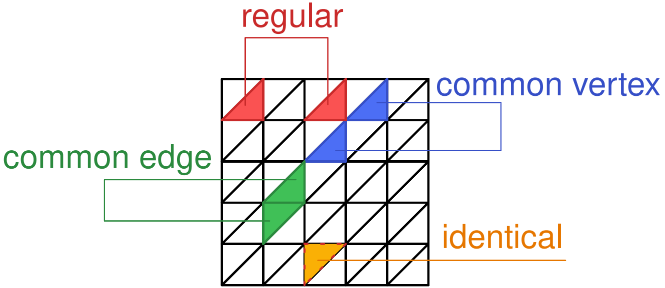
1. $[\mathbf{C}]_{i,j}$ involves integration of singular functions
2. $\mathbf{C}$ is dense, of size DOFs×DOFs
   - storage is expensive
   - matrix-vector product is also expensive
3. eigen solver

Solutions

1. Schauter-Schwab quadrature to alleviate singularity
2. hierarchical matrices
3. Thick-restart Lanczos

SCHAUTER-SCHWAB QUADRATURE

$$[\mathbf{C}]_{i,j} = \int_D \phi_j(\mathbf{x}) \int_D c(\mathbf{x},\mathbf{y})\phi_i(\mathbf{y})\, d\mathbf{y}\, d\mathbf{x}$$



SCHAUTER-SCHWAB QUADRATURE

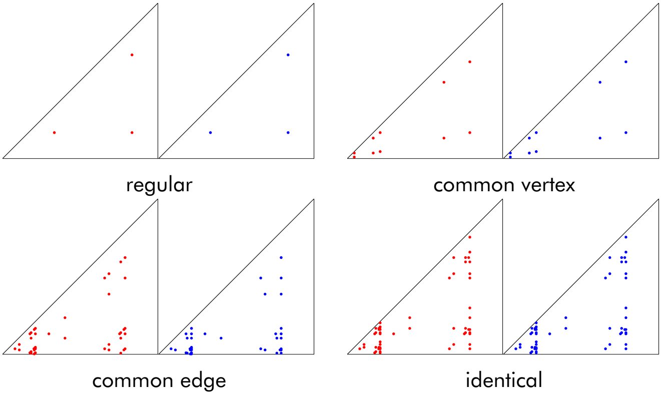


Fig. 18: Quadrature scheme for 4 different singularity cases

HIERARCHICAL MATRICES

Low-rank approximation of far-field blocks

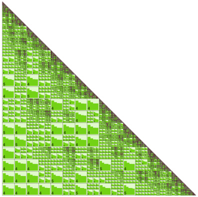


Fig. 19: Structure of a Hierarchical matrix

HIERARCHICAL MATRICES

Low-rank approximation of far-field blocks

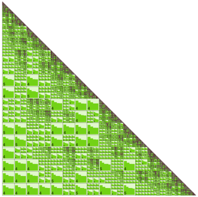


Fig. 19: Structure of a Hierarchical matrix

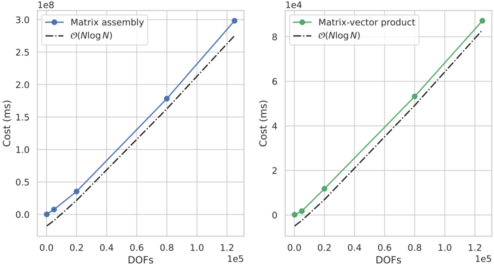


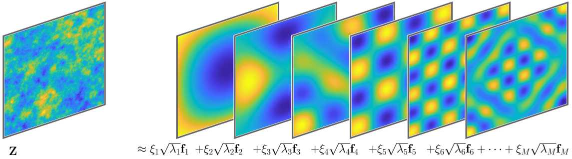
Fig. 20: Cost in terms of doing matrix assembly and matrix-vector product is reduced to $\mathcal{O} N \log N$ from N^2

MINIMAL BUT COMPLETE DEMO

```
#include <kleme.h>
int main(int argc,char **argv)
{
  // parse mesh
  kleme::Mesh mesh(argv[1]);

  // define dofhandler to handle mesh and basis function
  kleme::DofHandler dofhandler(mesh, 0);

  // create and assemble mass matrix
  kleme::Mass m_matrix(&dofhandler);
  m_matrix.assemble_matrix();

  // prepare quadrature rule and kernel for later use
  // in assembling stiffness matrix
  kleme::Quadrature quad(mesh.get_dim(), 2);
  kleme::ExponentialKernel kernel(1, 0.1, 45, 0.5);

  // create and assemble stiffness matrix
  kleme::StiffnessHmatrix k_hmatrix(&dofhandler, &kernel, &quad);
  k_hmatrix.assemble_matrix();

  // create solver
  kleme::SLEPc_Solver solver_hmatrix(&k_hmatrix, &m_matrix);
  int no_of_eigens = 100;
  solver_hmatrix.solve(no_of_eigens);

  // postprocess
  kleme::Postprocess postprocess(&dofhandler);
  postprocess.write_vtk(slepc_solver.eigen_vectors, "slepc_eigens.vtk");

  return 0;
}
```

CONCLUSIONS

- techniques behind `kleme`
- will be released to the public soon.
- drop me an email at **chao.zhang@math.tu-chemnitz.de** for early access



Thanks!

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BUNDESGESELLSCHAFT FÜR ENDLAGERUNG

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