Uncertainties in THM-coupled integrity calculations

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OUTLINE

Parameter uncertainity in THM process – Feliks

Inhomogeneity and anisotropy in THM simulations – Aqeel

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

INTRODUCTION

Goals:

- Investigate if combining experimental data with modelling allows to gain insight to the effect of the thermo-osmosis process has impact on the pressurization.
- If an impact can be detected, quantify how big it is -> parameter estimation.

Uncertainities

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

What is thermo-osmosis?

TO is defined as follows:
"*Thermo-osmosis may be defined as the process of diffusion of a fluid through a membrane under the influence of a temperature gradient*" (Denbigh et al. 1952), (Gonçalvès et al. 2018)

- 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

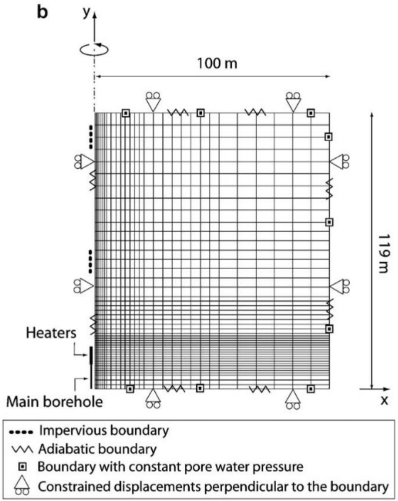


Fig. 1: Layout of ATLAS Experiment. Figure from: François et al. 2009

UNCERTAINTY QUANTIFICATION WORKFLOW

- Proxy building: parameter space was explored using numerical simulations based on Latin Hypercube Sampling (LHS) and 2-level-full-factorial experiment design
- Monte Carlo combined with proxies were used to explore parameter space with high saturation

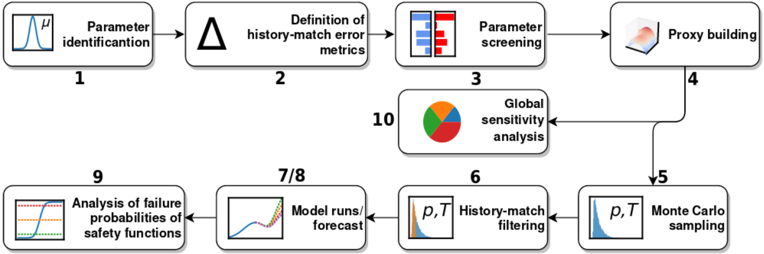


Fig. 2: Overview of the workflow used in this study. J. Buchwald et al. 2020

HYPOTHESIS TESTING

Goals:

- Test if TO has more impact than just being an arbitrary tweaking parameter
- Test if numerical method allow to select correct physical process
- Investigate how well the correct parameters can be recovered

Tab. 1: Table presenting an overview of tested process hypothesis. Each hypothesis is combination of a selection of a physical process and how thermo-osmosis is added to process. **Bold hypothesis** is the correct hypothesis in first experiment with no thermo-osmosis in reference data, *hypothesis in italics* is the correct hypothesis in the second experiment in which thermo-osmosis was included in the reference data.

Process \ TO status	no TO	with TO	with TO active
THM	**THM**	*THM+TO*	*THM+TO_active*
TRuni	TRuni	TRuni+TO	TRuni+TO_active
TRhyd	TRhyd	TRhyd+TO	TRhyd+TO_active

SIMULATION SETUP

Tested parameter ranges

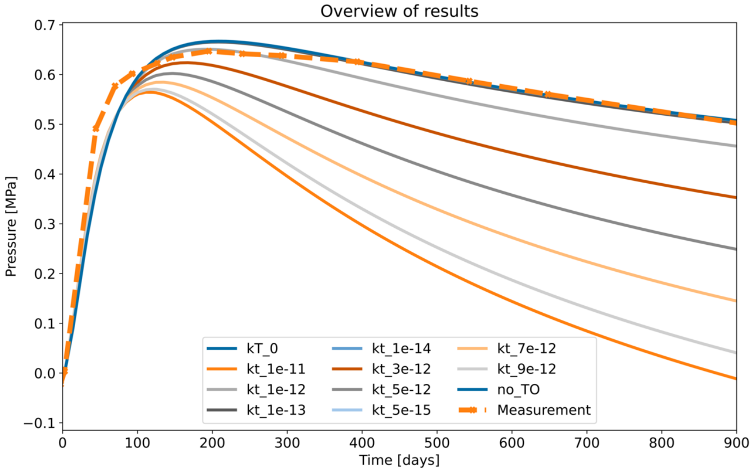
Parameter name	Unit	Reference	Min	Max
Intrinsic permeability (k)	m^2	$2.5e-19$	$1e-19$	$9e-19$
TO coefficient (narrow) (k_T)	$\mathrm{Pa} * \mathrm{m} * \mathrm{K}^{-1}$	$3e-12$	$1e-12$	$5e-12$
TO coefficient (wide) (k_T)	$\mathrm{Pa} * \mathrm{m} * \mathrm{K}^{-1}$	$3e-12$	$1e-14$	$1e-11$
Young's modulus (E)	Pa	$3.5e8$	$2e8$	$8e8$

Error metrics - History matching error:

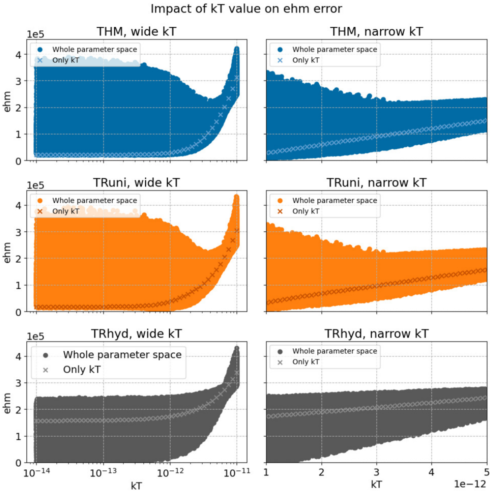
$$e_{HM} = \sqrt{\sum_{1}^{n} \frac{(d_{obs} - d_{sim})^2}{n}} \tag{1}$$

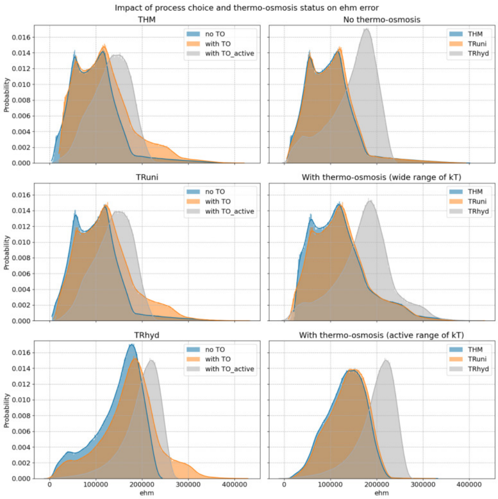
Parameters and initial conditions after: (Tamizdoust et al. 2021).

IMPACT OF THE VALUE OF K_T - TO COEFFICIENT

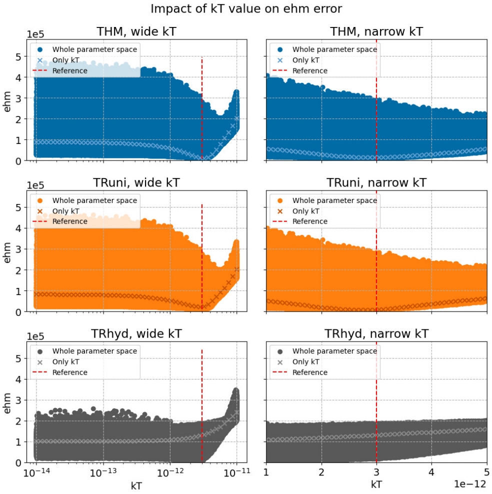


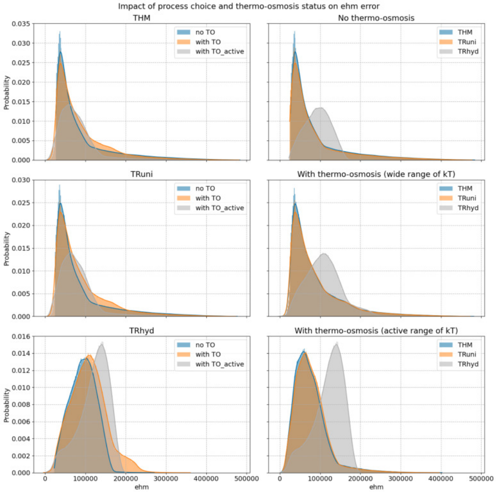
DISTRIBUTION OF ERROR VALUES - NO TO IN REFERENCE



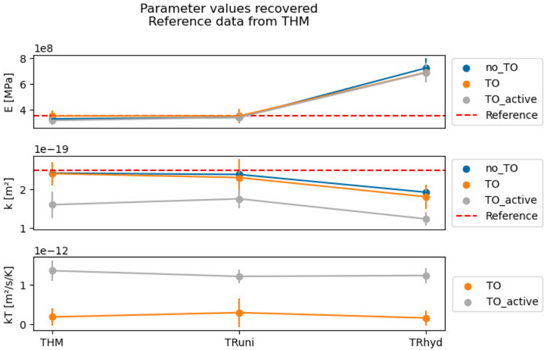


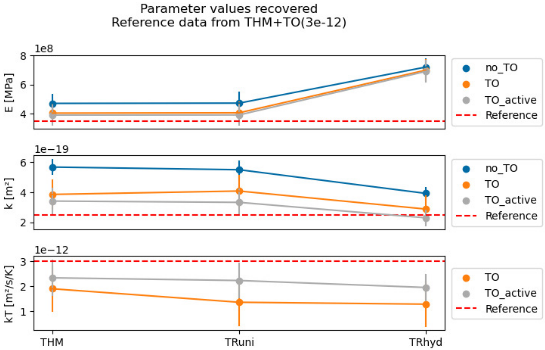
DISTRIBUTION OF ERROR VALUES - WITH TO IN REFERENCE





ESTIMATED PARAMETERS





DISTRIBUTION OF PARAMETER VALUES

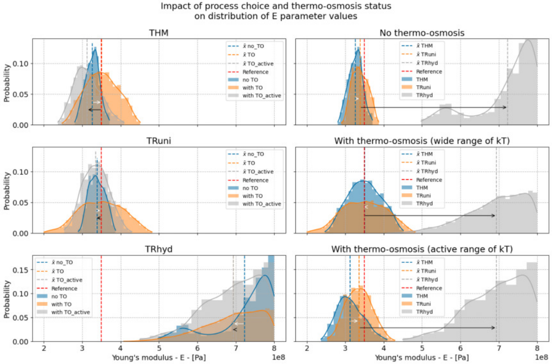


Fig. 3: Distribution of E values recovered with different processes with TO_active. No TO in the reference data.

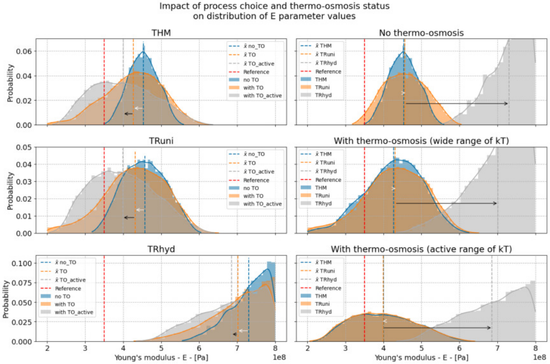


Fig. 4: Distribution of E values recovered with different processes with TO_active. With TO in the reference data.

DISTRIBUTION OF PARAMETER VALUES

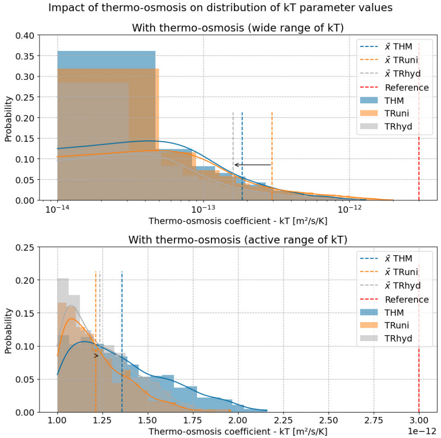


Fig. 5: Distribution of kT recovered with different processes with TO_active. No TO in the reference data.

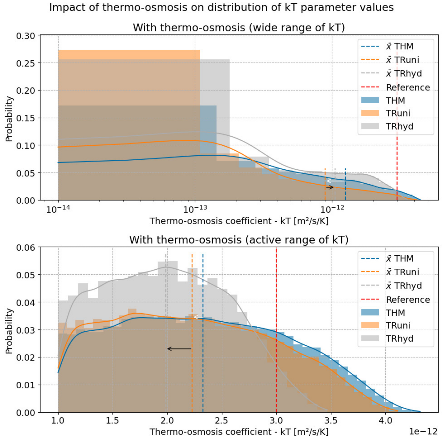


Fig. 6: Distribution of kT recovered with different processes with TO_active. With TO in the reference data.

SUMMARY AND OUTLOOK

Summary and conclusions:

- Increasing the complexity of the model doesn't necessarily improve the result
- The UQ tools can be used to discriminate between processes, select parameter values and quantify uncertainty

Outlook:

- Add information from multiple observations points
- Repeat the study presented in this presentation using data from real waste storage experiment
- Verify the significance of difference between the recovered distributions of parameter values with statistical methods

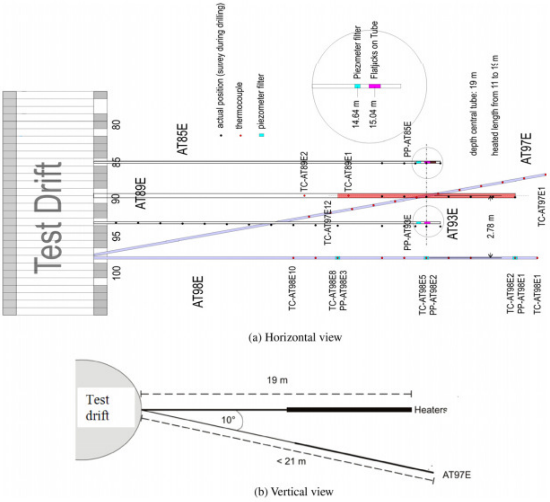
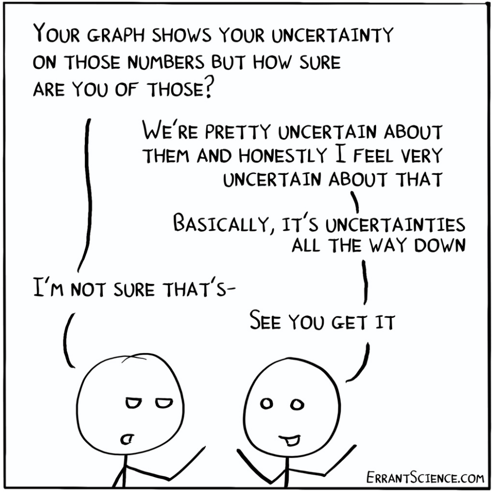


Fig. 1. Schematic view with instrumentation of the ATLAS III in situ test.

Fig. 7: ATLAS experiment - sensor positions (Chen et al. 2011

COMICAL RELIEF AT THE END OF PRESENTATION :)



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 <–> intrinsic permeability)

What's new?

- Extension to other parameters like E, λ, α_s, c_p, ϕ
- Departure from rectangular to circular geometry
- Extension of plots to two more measures
- Spatial percentile plots

Governing equations – TRM (Pitz et al. 2023)

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:

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

Momentum balance:

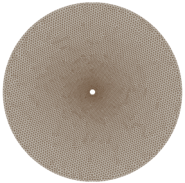
$$\operatorname{div}\left(\boldsymbol{\sigma}^{\text{eff}} - \alpha_{\text{B}} \chi(S_{\text{L}}) p_{\text{LR}}\, \mathbf{I}\right) + \rho \mathbf{g} = \mathbf{0}$$

with

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

Model setup and specifics

- Simplified 2D mesh: $r = 50\,\mathrm{m}$
  –> host rock (Opalinus clay)
- Circular heat source of $r = 1.5\,\mathrm{m}$
  –> 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:
$T_0 = 15\,°\mathrm{C}$, $p_0 = 2\,\mathrm{MPa}$, $u_{S0} = 0$

Boundary conditions:

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

CASE STUDIES

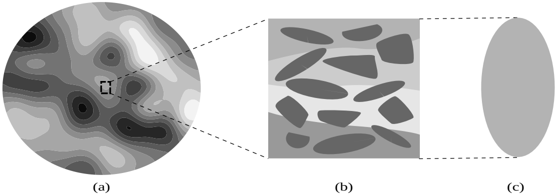
–> Let f be the parameter in question
–> f in this study –> λ, k, E
–> $f_\perp = a_f \, f_{||}$, where a_f is a scaling factor

- Homogeneous, isotropic
  –> $f_x = f_y = f_{||}$
- Homogeneous, anisotropic
  –> $f_x = f_{||}, \quad f_y = f_\perp$
- Heterogeneous, statistically isotropic, hydraulically isotropic
  –> $f_x(\text{RF}) = f_y(\text{RF}) = f_{||}$
- Heterogeneous, statistically isotropic, hydraulically anisotropic
  –> $f_x(\text{RF}) = f_{||}, \quad f_y(\text{RF}) = f_\perp$

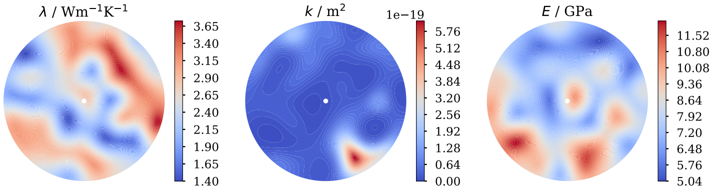
Work in progress

- Heterogeneous, statistically anisotropic, hydraulically isotropic
  –> $f_x(\text{RF}_x) = f_{||}, \quad f_y(\text{RF}_y) = f_{||}$
- Heterogeneous, statistically anisotropic, hydraulically anisotropic
  –> $f_x(\text{RF}_x) = f_{||}, \quad f_y(\text{RF}_y) = f_\perp$

- Basic concept of the study

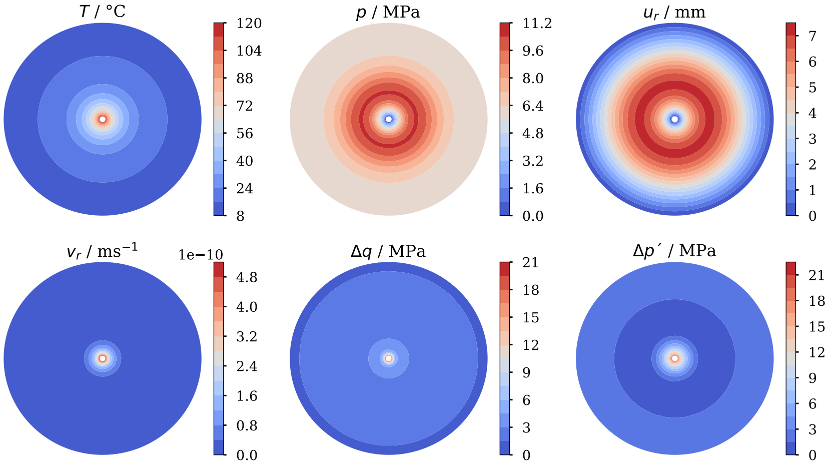


- Example of one random realisation



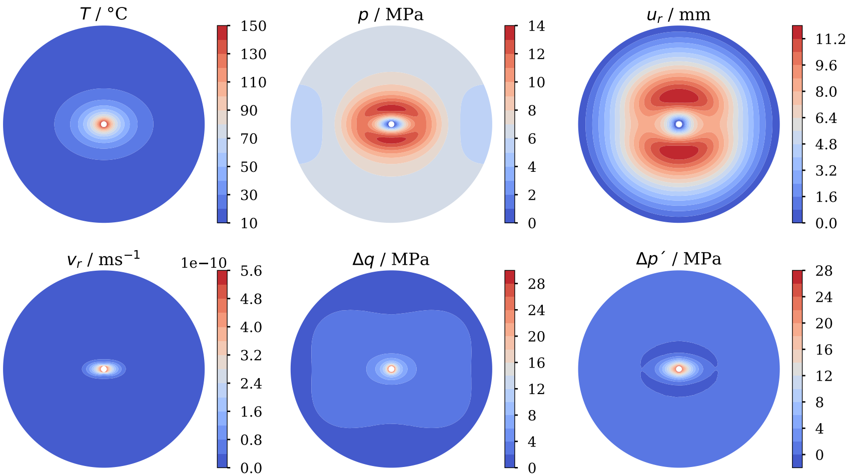
–> $\Delta q = \sqrt{\frac{3}{2}\sigma'_\mathrm{d} : \sigma'_\mathrm{d}}$ $\Delta p' = -\frac{1}{3}\sigma'_{ii}$

Homogeneous, isotropic (reference) case

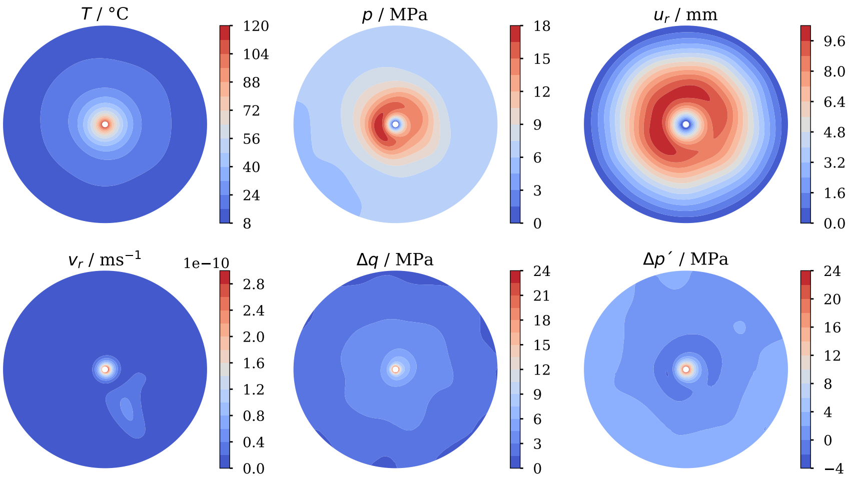


Inhomogeneity and anisotropy in THM simulations – Aqeel

Homogeneous, anisotropic case



Heterogeneous, isotropic (single case)



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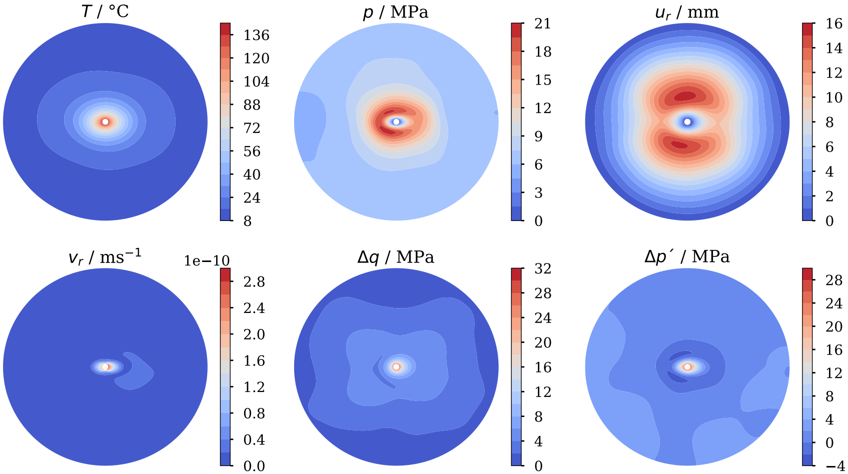
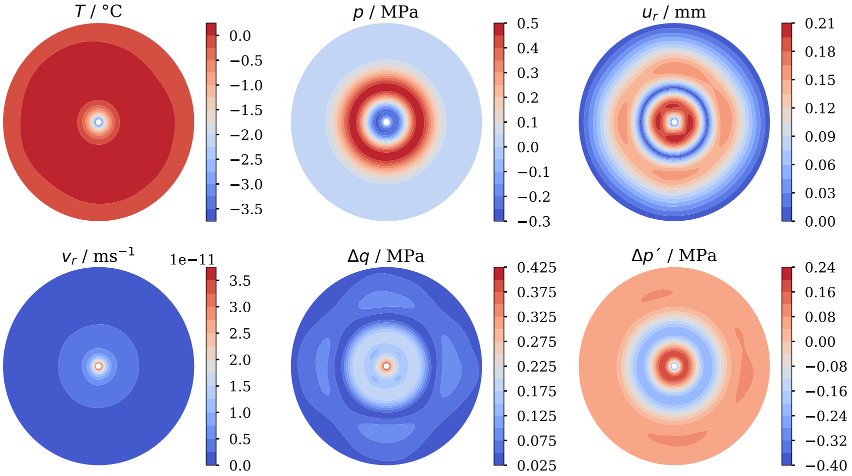
Heterogeneous, anisotropic (single case)



Diff. between hom. iso and mean of het. isotropic (needed?)



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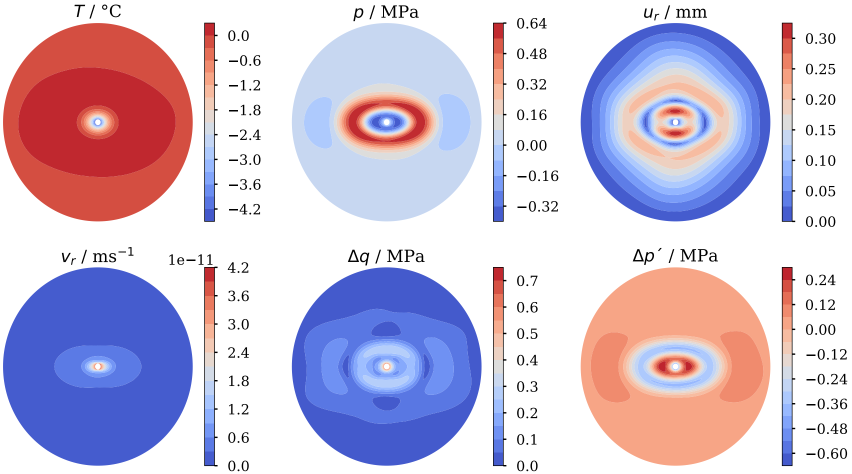
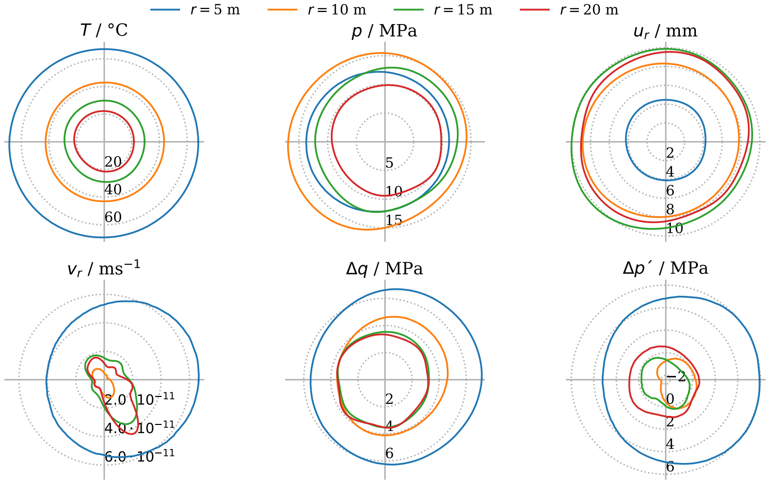


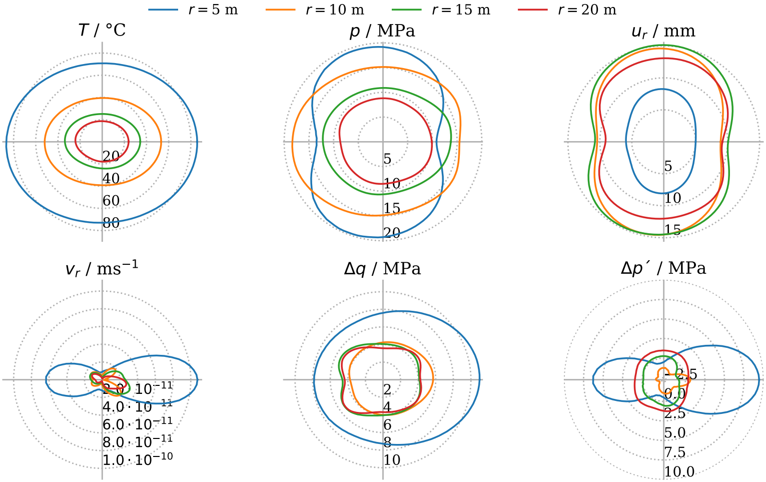
Inhomogeneity and anisotropy in THM simulations – Aqeel

Heterogeneous, isotropic (single case)

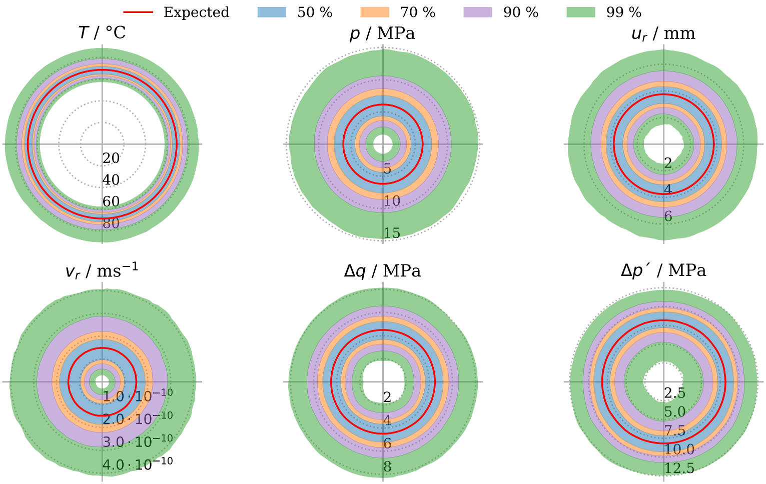


Inhomogeneity and anisotropy in THM simulations – Aqeel

Heterogeneous, anisotropic (single case)

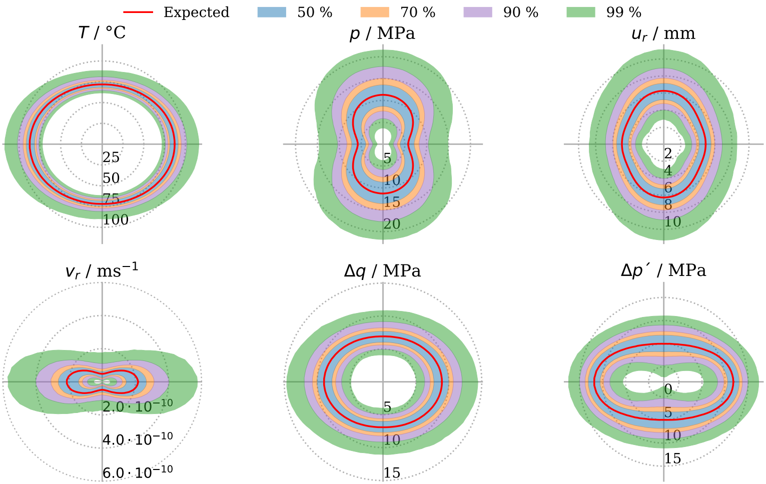


Heterogeneous, isotropic, percentiles at $r = 5\,\mathrm{m}$



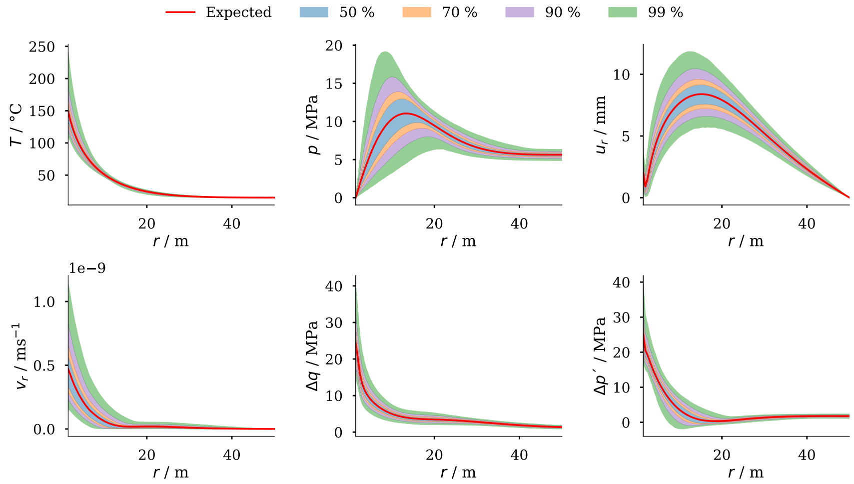
Inhomogeneity and anisotropy in THM simulations – Aqeel

Heterogeneous, anisotropic, percentiles at $r = 5\,\mathrm{m}$



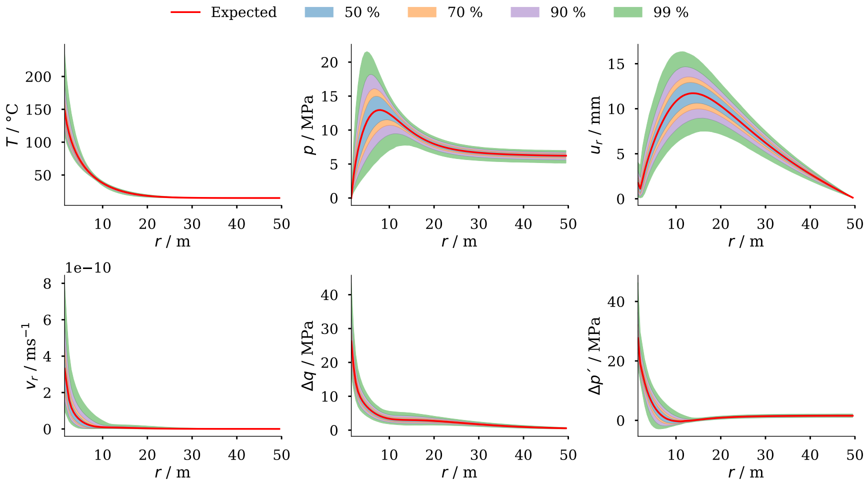
Inhomogeneity and anisotropy in THM simulations – Aqeel

Heterogeneous, anisotropic, percentiles at $\theta = 0°$

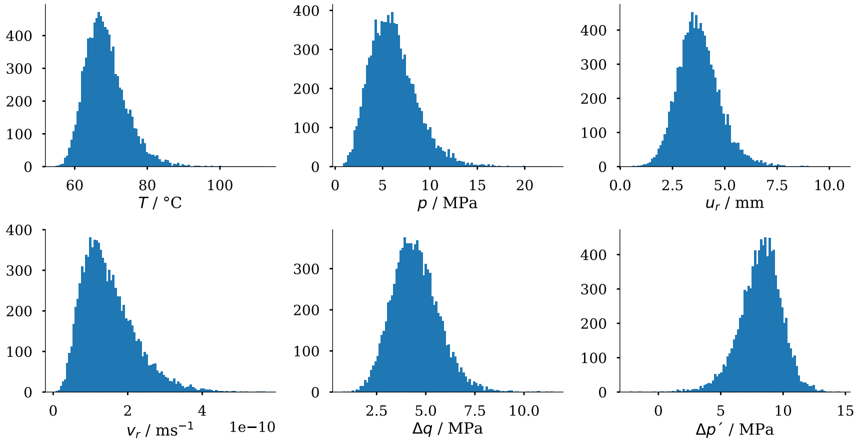


Inhomogeneity and anisotropy in THM simulations – Aqeel

Heterogeneous, anisotropic, percentiles at $\theta = 90°$



Heterogeneous, isotropic, histogram at $r = 5\,\mathrm{m}$ & $\theta = 0°$



Outlook

- Statistical anisotropy
  –> Different correlation lengths
- Random anisotropy
  –> $f_\perp \neq a_f \, f_{||}$?
- Different boundary conditions (?)
- Unsaturated settings (?) (complex)
- Better ways to interpret results?
- Additional runs for min, mean, max for all 3 inputs

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BUNDESGESELLSCHAFT FÜR ENDLAGERUNG

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OUTLINE

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

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

KARHUNEN-LOÈVE EXPANSION (KLE)

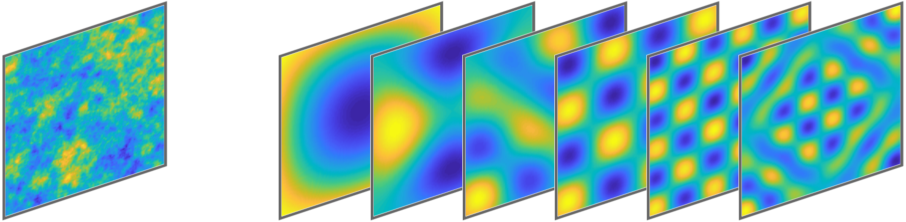
$$\mathbf{Z}(\mathbf{x},\xi) \approx \sum_{i=1}^{M} \xi_i \sqrt{\lambda_i}\mathbf{f}_i(\mathbf{x})$$

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

KARHUNEN-LOÈVE EXPANSION (KLE)

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

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

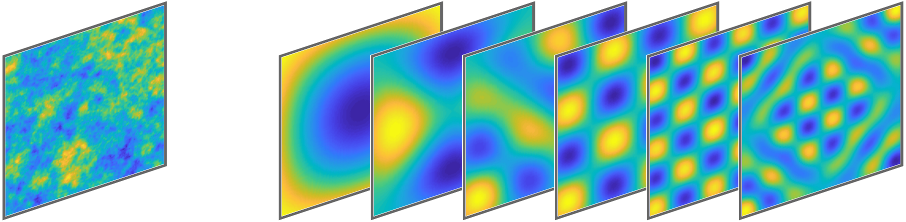


$$\mathbf{Z} \approx \xi_1\sqrt{\lambda_1}\mathbf{f}_1 + \xi_2\sqrt{\lambda_2}\mathbf{f}_2 + \xi_3\sqrt{\lambda_3}\mathbf{f}_3 + \xi_4\sqrt{\lambda_4}\mathbf{f}_4 + \xi_5\sqrt{\lambda_5}\mathbf{f}_5 + \xi_6\sqrt{\lambda_6}\mathbf{f}_6 + \cdots + \xi_M\sqrt{\lambda_M}\mathbf{f}_M$$

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 $\mathcal{N}(0, 1)$



$\mathbf{Z}$ $\approx \xi_1\sqrt{\lambda_1}\mathbf{f}_1 + \xi_2\sqrt{\lambda_2}\mathbf{f}_2 + \xi_3\sqrt{\lambda_3}\mathbf{f}_3 + \xi_4\sqrt{\lambda_4}\mathbf{f}_4 + \xi_5\sqrt{\lambda_5}\mathbf{f}_5 + \xi_6\sqrt{\lambda_6}\mathbf{f}_6 + \cdots + \xi_M\sqrt{\lambda_M}\mathbf{f}_M$

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

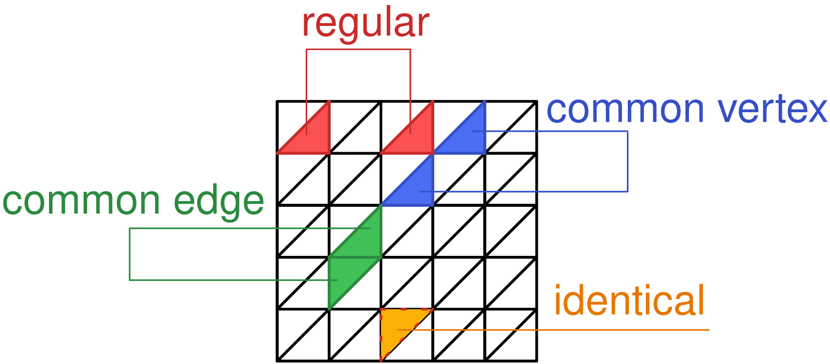
1. $[\mathbf{C}]_{i,j}$ involves integration of singular functions, i.e., $c(|\mathbf{x}-\mathbf{y}|)$
2. $\mathbf{C}$ is dense, of size DOFs$\times$DOFs
   - storage is expensive
   - matrix-vector product is also expensive
3. eigen solver

Solutions

1. Schauter-Schwab quadrature from the BEM community 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

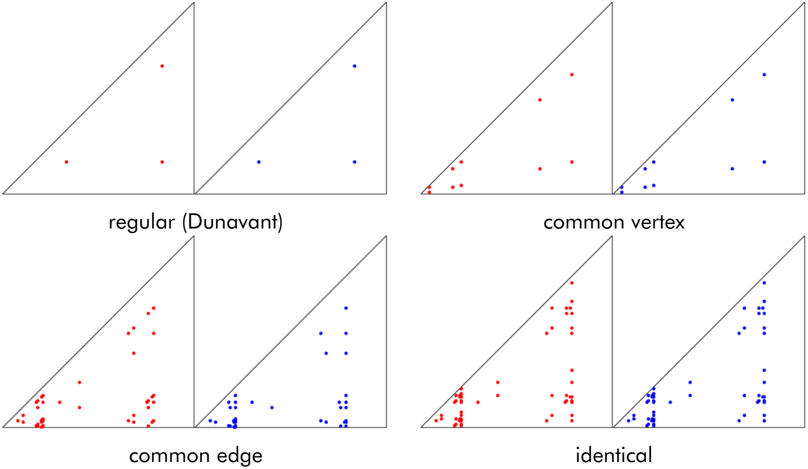


Fig. 9: Quadrature scheme on reference element pairs for 4 different cases

HIERARCHICAL MATRICES

Low-rank approximation of far-field blocks

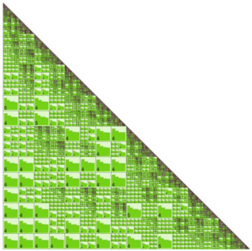


Fig. 10: Structure of a Hierarchical matrix

HIERARCHICAL MATRICES

Low-rank approximation of far-field blocks

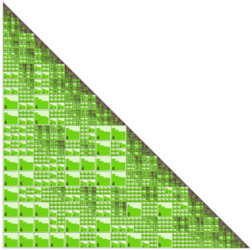


Fig. 10: Structure of a Hierarchical matrix

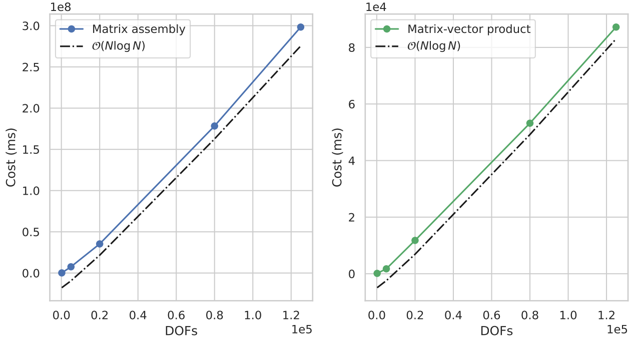


Fig. 11: Cost in terms of doing matrix assembly and matrix-vector product is reduced to $\mathcal{O}N \log N$ from N^2

CODE STRUCTURE

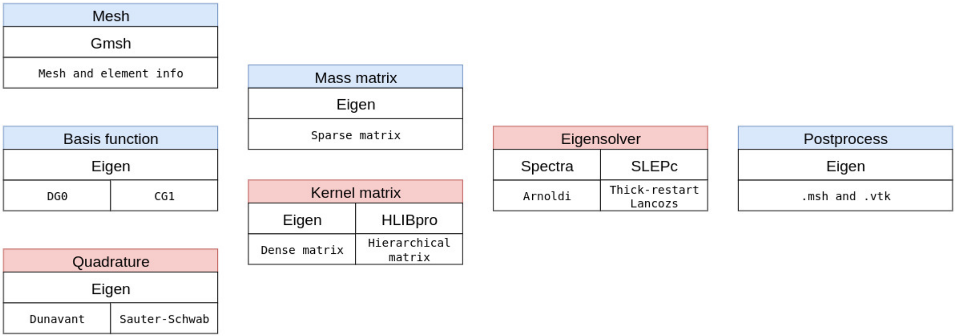


Fig. 12: Code structure

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;
}
```

DOXYGEN DOCUMENTATION

kleme 0.3
Karhunen–Loève expansion made easy

Main Page | Related Pages | Namespaces | Classes | Files | Search

- kleme
  - Example
  - Common use
  - **Code structure**
  - Performance
  - Highlights
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  - License
  - todo
  - Namespaces
  - Classes
  - Files

kleme Documentation

kleme stands for **K**arhunen–**L**oève **e**xpansion **m**ade **e**asy. It is a C++ library for solving the integral eigen-value problem (IEVP) from discretizing the kernel operator with the Galerkin method.

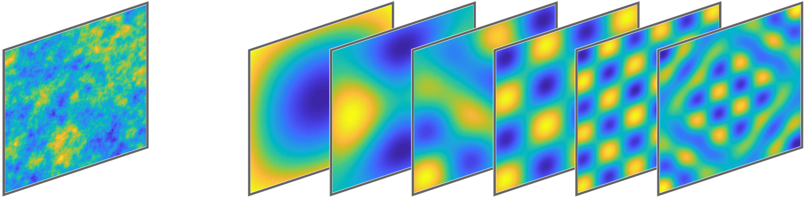
Example

```cpp
#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");
```

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

CONCLUSIONS

- theories and techniques behind `kleme`
- demonstration of the use
- working on further improvement of internal data structure and documentation



$$\mathbf{Z} \approx \xi_1\sqrt{\lambda_1}\mathbf{f}_1 + \xi_2\sqrt{\lambda_2}\mathbf{f}_2 + \xi_3\sqrt{\lambda_3}\mathbf{f}_3 + \xi_4\sqrt{\lambda_4}\mathbf{f}_4 + \xi_5\sqrt{\lambda_5}\mathbf{f}_5 + \xi_6\sqrt{\lambda_6}\mathbf{f}_6 + \cdots + \xi_M\sqrt{\lambda_M}\mathbf{f}_M$$

Thanks!