Characterization of spatial heterogeneity of geomaterials in large scale groundwater bodies through a compositional data approach

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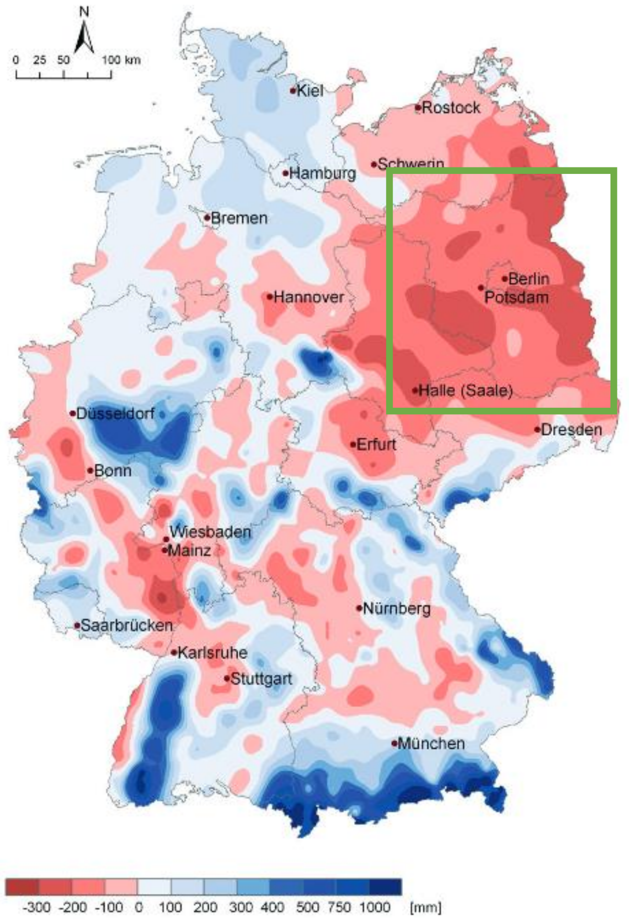
Water scarcity in Germany

2041-2050



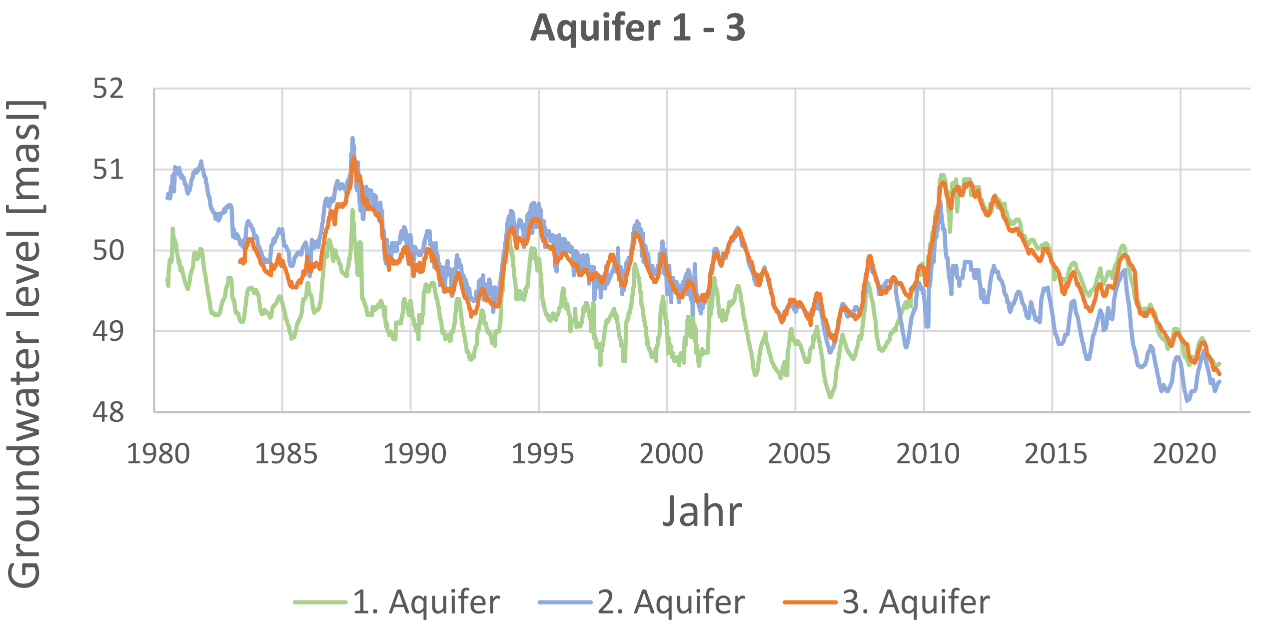
Climatic water balance © PIK, 2013

Is there enough water left?

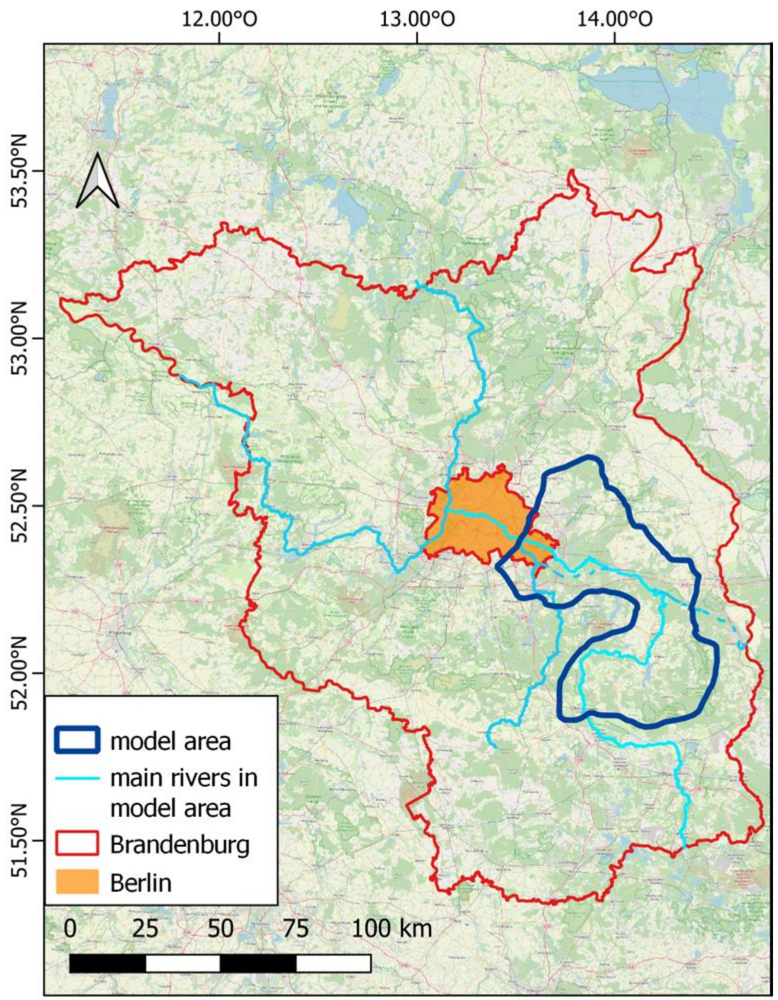
- Decreasing groundwater recharge expected
- Dropping groundwater levels

➡ Increasingly tense water situation

Need for large scale groundwater model



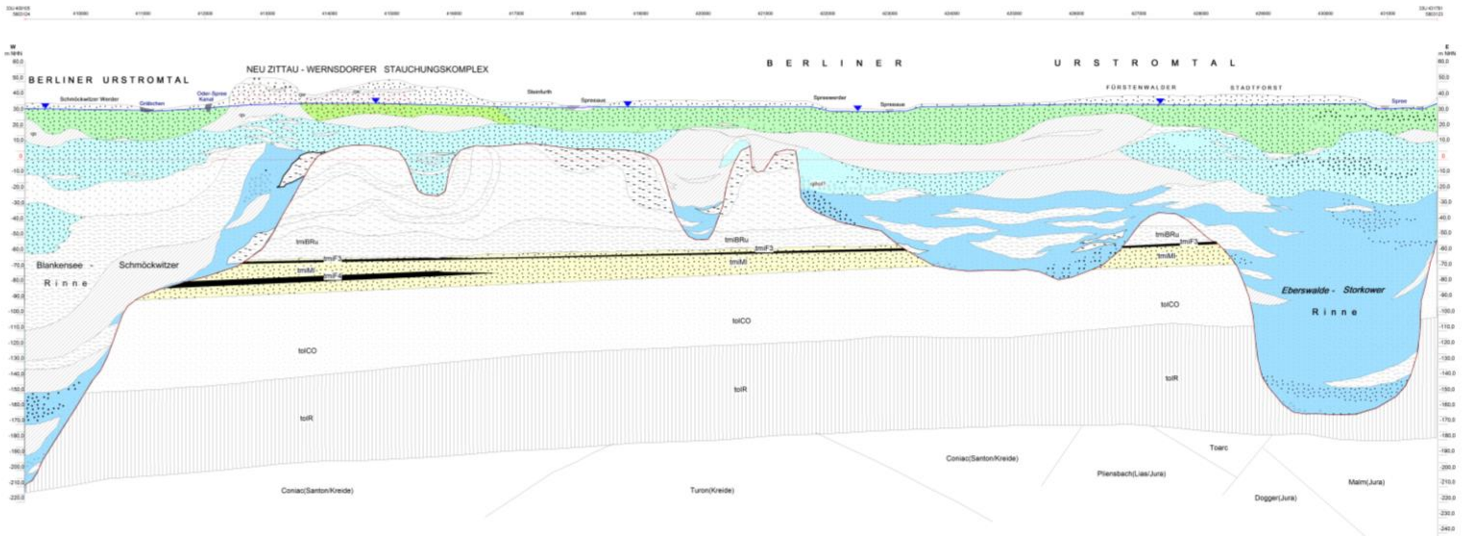
Model area



Model area in Brandenburg

The complexity of Brandenburs geology

- **Large scale** model → area 3400 km²
- 200 m depth → 3 individual aquifers



Hydrogeolical cross section in the model area © LBGR, 2001

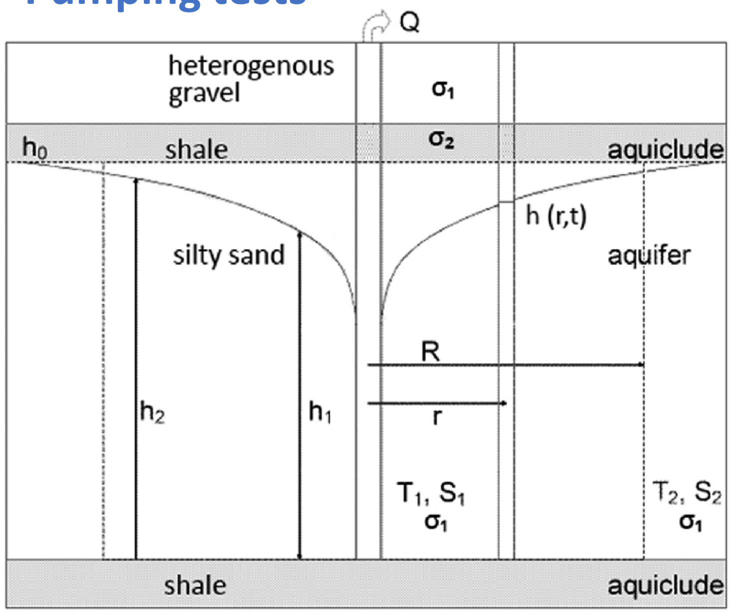
- Highly **complex** and heterogeneous **geology**
- Highly discontinuous layering prone to **numerical instabilities**

Parameters: Blessing and Curse

Groundwater flow is defined by hydraulic parameter

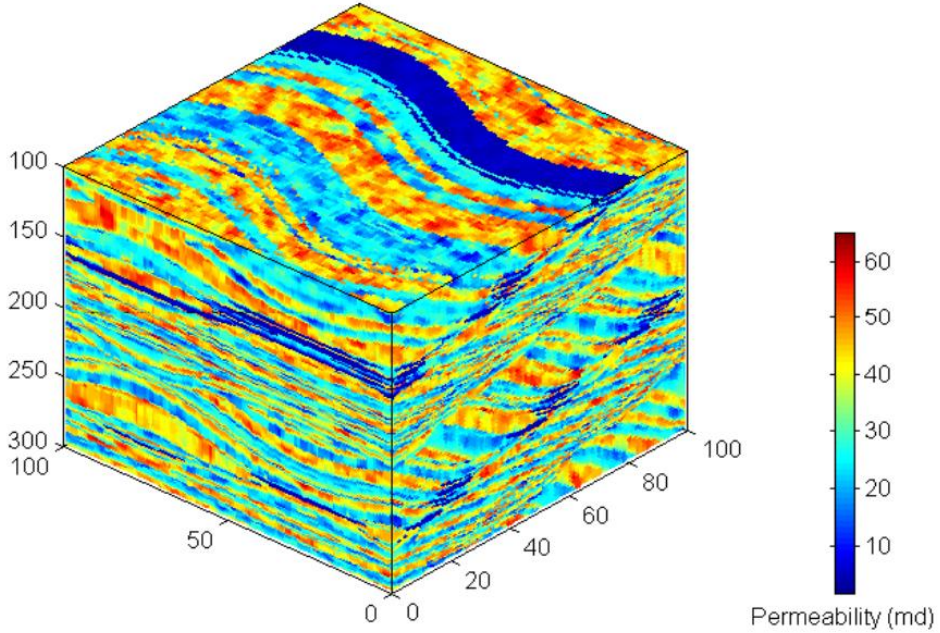
$$\frac{\partial}{\partial x}\left(K_x\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial h}{\partial z}\right)+q_s=S_s\frac{\partial h}{\partial t}$$

Pumping tests



Sketch of pumping test [Oliveti & Cardarelli, 2017]

Interpolation

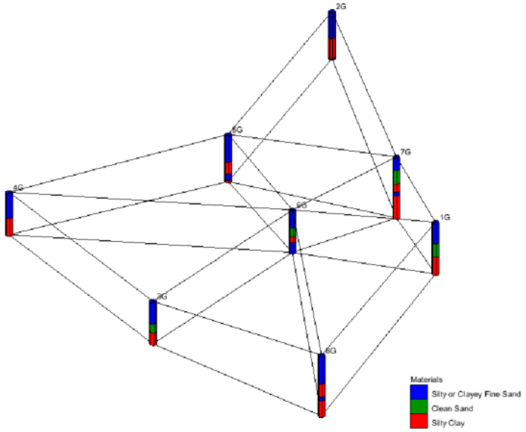


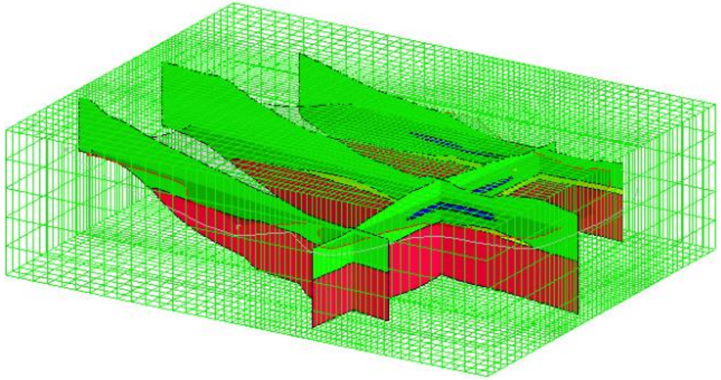
Discrete distribution of continuous variable, modified after Dubrule & Damsleth, 2001

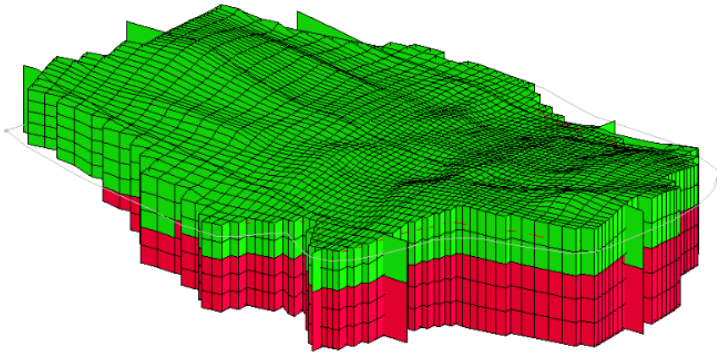
… a potential way out?

Borehole core samples © BBB, 2014

- Interpolation of materials based on bore hole information
- Often done on a layer basis → materials are required to be clustered
  - ➢ Easy to calibrate
  - ➢ No heterogeneity/loss of information





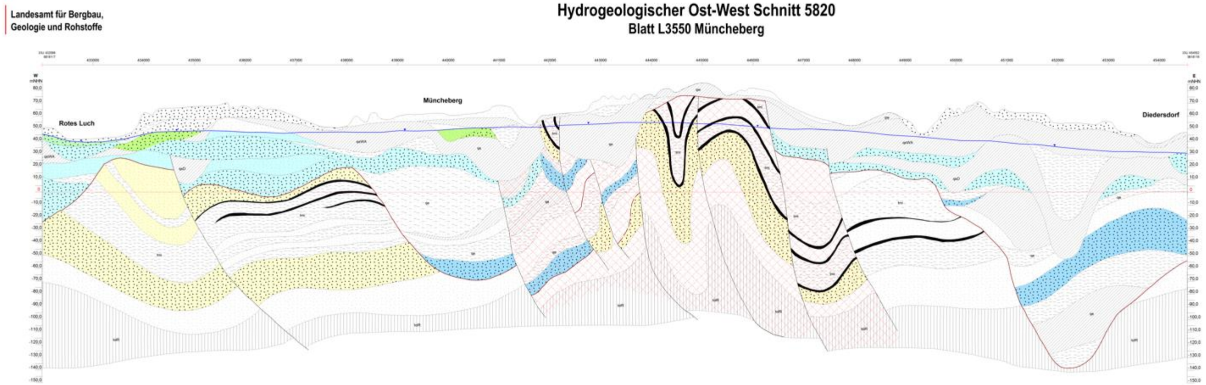


Interpolation by layer construction based on borehole data © AQUAVEO

Large scale or small scale… why not both?

Regional flow

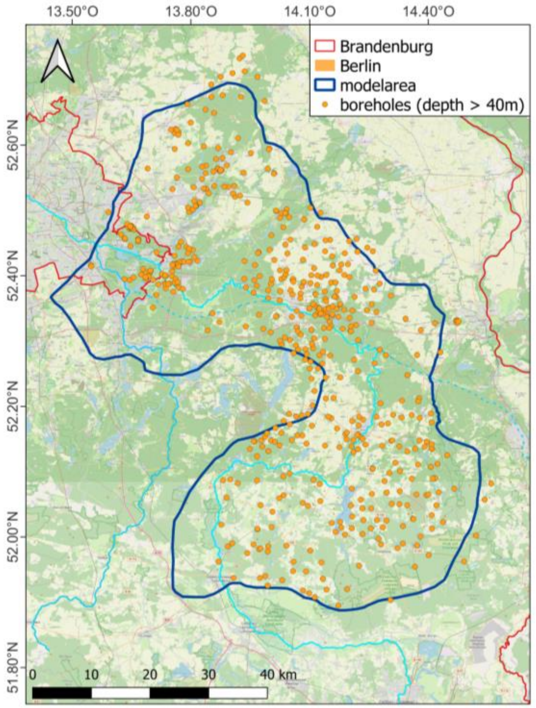
- Determined by hydrogeological layers
- Rough material classes
- Based on hydrogeological cross sections



Hydrogeological cross section for Brandenburg region © LBGR, 2001

Local flow

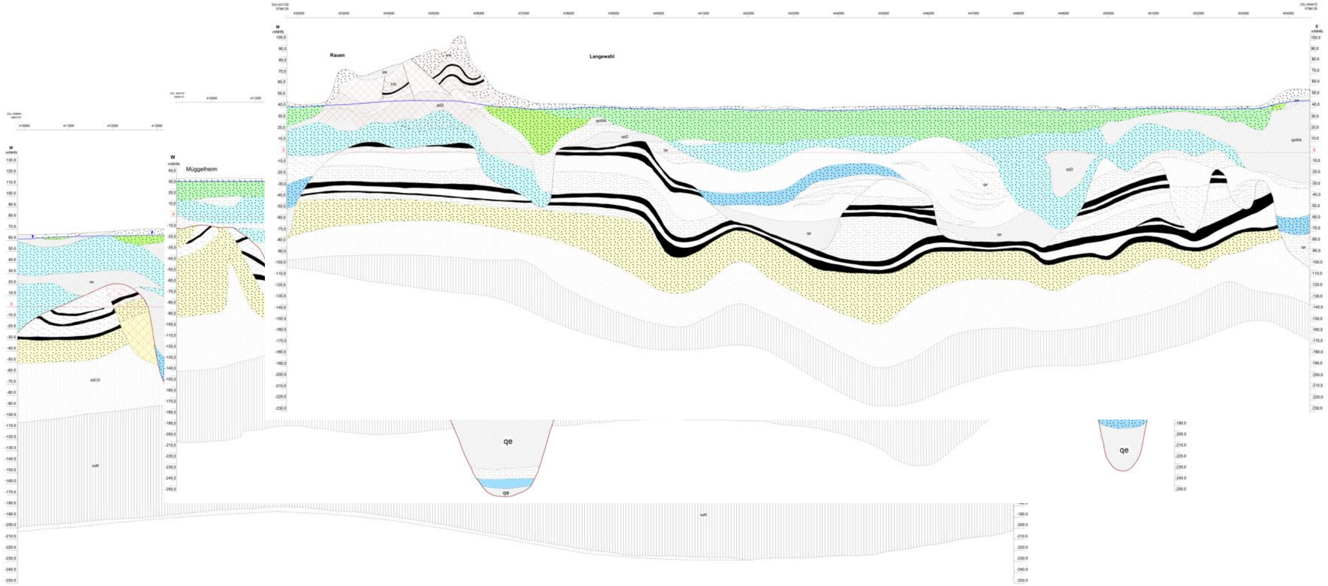
- Determined by material heterogeneities
  - More detailed soil information required
- Based on borehole data



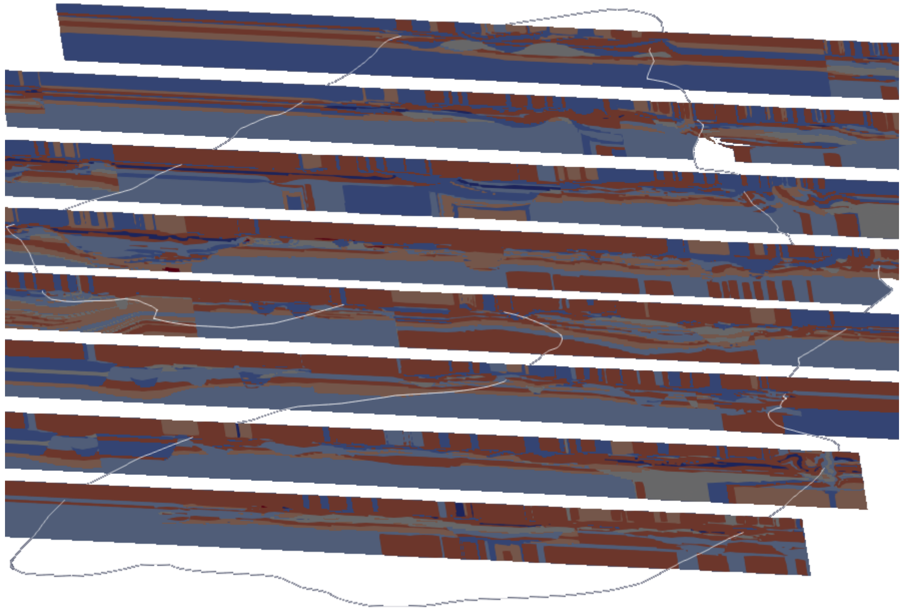
Model area and locations of boreholes deeper than 40 m

Coarse interpolation for coarse data…

- Hydrogeological layers are seen as macrounits
- coarse interpolation method → deterministic k nearest neighbor
- Define the domain for the second interpolation step



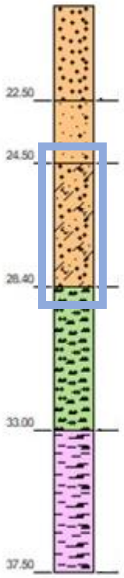
Hydrogeolical cross section in the model area © LBGR, 2001



Digitized hydrogeolical cross section in the model area

… and refined interpolation for fine data!

- **Introduce** material **heterogeneities** within each material
- **Performed within domains** from first interpolation step
  - predetermined domain of similar materials **aids** in satisfaction of **stationarity**



S; u4, t2

Sand, which is strongly silty and slightly clayey

60% sand

30% silt

10% clay

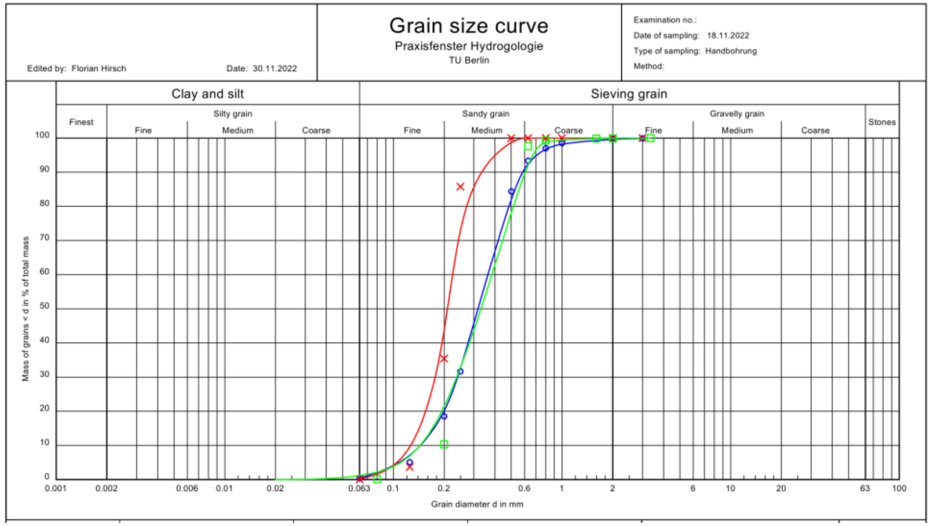
Borehole data © GeODin

$$K = \beta C d_{10}^2, \qquad K = \beta \frac{g}{v} \frac{n^3}{(1-n)^2} d_{17}^2$$

$$S = 6(1-n)/d_H$$

$$\alpha_L = \gamma d_{50}$$

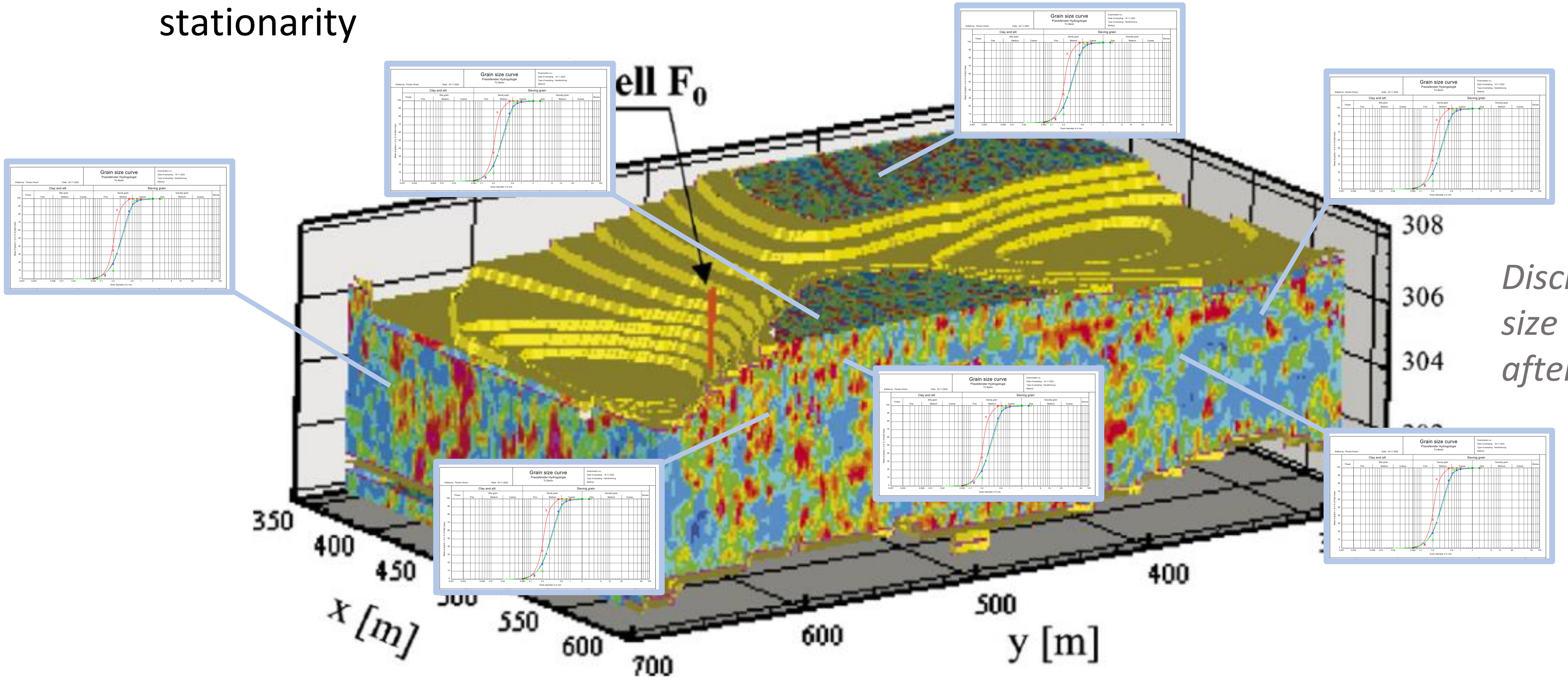
$$D \sim Pe^n = \left(\frac{v d_{50}}{D_m}\right)^n$$



Example of a grain size distribution curve

… and refined interpolation for fine data!

- Introduce material heterogeneities within each material
- Performed within domains from first interpolation step
    - predetermined domain of similar materials aids in satisfaction of stationarity



Discrete distribution of grain size distributions, modified after Riva et al., 2006

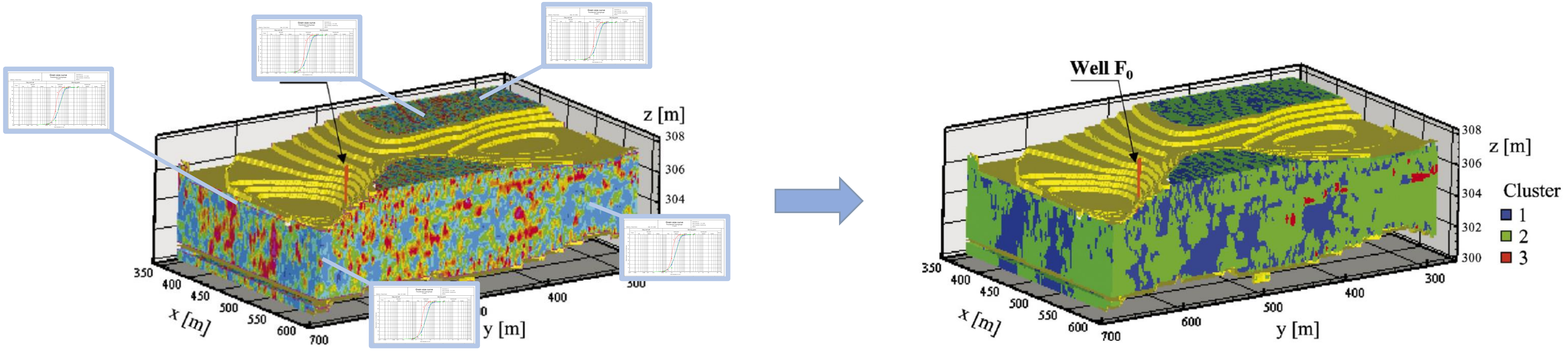
Compositional data approach

The peculiarity with compositional data

- Grain size distribution adds up to 1
  - Compositional data → $\begin{bmatrix} sand \\ silt \\ clay \end{bmatrix} = \begin{bmatrix} 0.6 \\ 0.3 \\ 0.1 \end{bmatrix}$

Standard statistics do not work anymore!
→ compositional kriging

Clustering of interpolated grain size distributions holds geological meaning



Conversion of continuous to clustered data, modified after Riva et al., 2006

Conclusion

- Domain interpolation aids with stationarity assumption
- We preserve higher degree of information
- Clustering adjustable and reproducible
- Grain size distributions allow for estimation of various parameters
- Clusters hold geological meaning

Thank you for your attention!

Grainsizes

Compositional vector: $\begin{bmatrix} decris/stones \\ coarse\ gravel \\ middle\ gravel \\ fine\ gravel \\ coarse\ sand \\ middle\ sand \\ fine\ sand \\ coarse\ silt \\ middle\ silt \\ fine\ silt \\ coarse\ clay \\ middle\ clay \\ fine\ clay \end{bmatrix} = \begin{bmatrix} 131.5 \\ 41.5 \\ 13.15 \\ 4.15 \\ 1.315 \\ 0.415 \\ 0.1315 \\ 0.0415 \\ 0.01315 \\ 0.00415 \\ 0.001315 \\ 0.000415 \\ 0.0001315 \end{bmatrix} mm$ → 13 classes