Radionuclide sorption in the far field: Geostatistical simulation of crystalline rock to assess uncertainties due to heterogeneities

Alexandra Duckstein, Solveig Pospiech, Raimon Tolosana-Delgado, and Vinzenz Brendler

Helmholtz-Zentrum Dresden-Rossendorf (HZDR) · Institute for Resource Ecology (IRE) · Alexandra Duckstein · a.duckstein@hzdr.de · www.hzdr.de
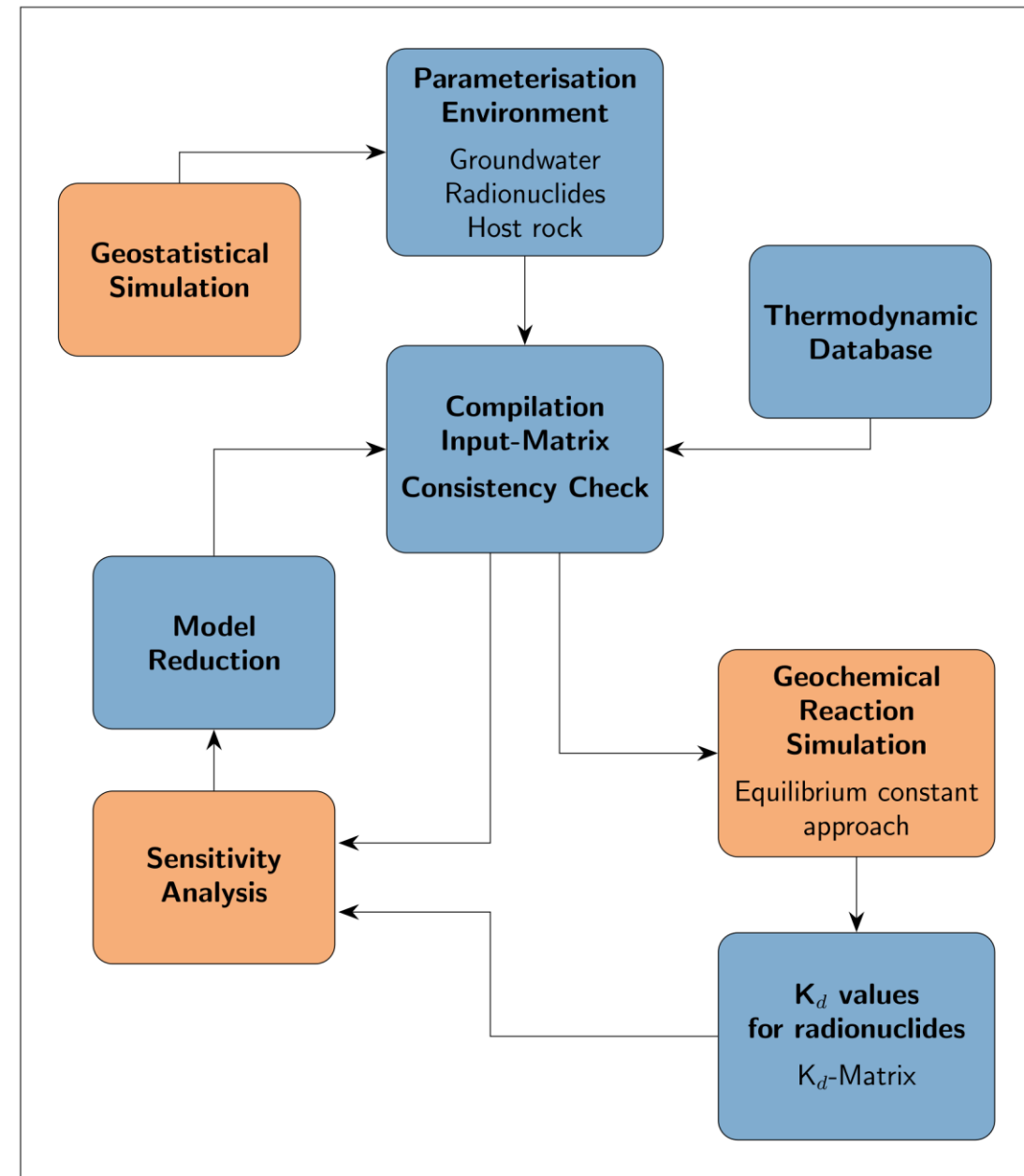
Research Context

SANGUR Project

- Handle heterogeneities in crystalline host rock by using geostatistical simulation
  - → many realizations

- Geochemical Reaction Simulation
  - → retardation of radionuclides

- Sensitivity Analysis
  - → strong/weak impact of model parameters

> SANGUR
> Systematic sensitivity analysis for mechanistic geochemical models using field data from crystalline rock

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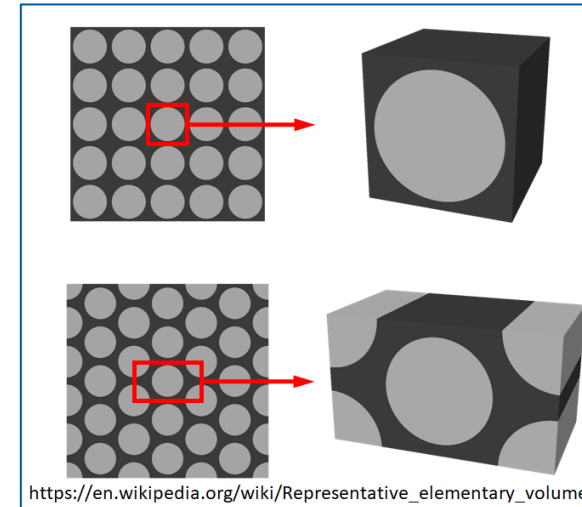
Research question addressed in this presentation

Determination of the optimum representative volume element

On which scale do we have to work?
What is the size of our optimal representative
volume element (RVE) in 2D?

- The size of our RVE should not affect the calculation of the distribution coefficient (K_d-value).
  - → Sensitivity analysis provides better information about system-describing parameters.
- Large enough to preserve the "statistics of the material",
- But small enough that it is still easy to "calculate".
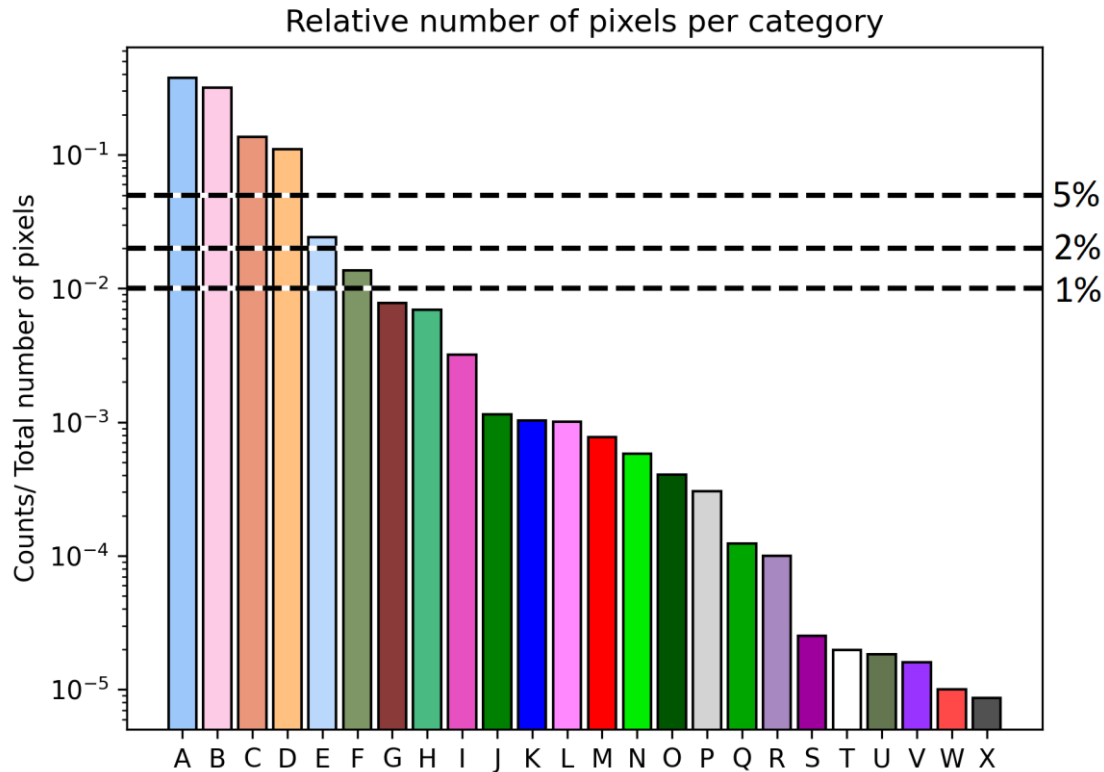
RVE
Representative Volume
Element

https://en.wikipedia.org/wiki/Representative_elementary_volume

Microstructure model that fully represents the inhomogeneity of the (crystalline) rock

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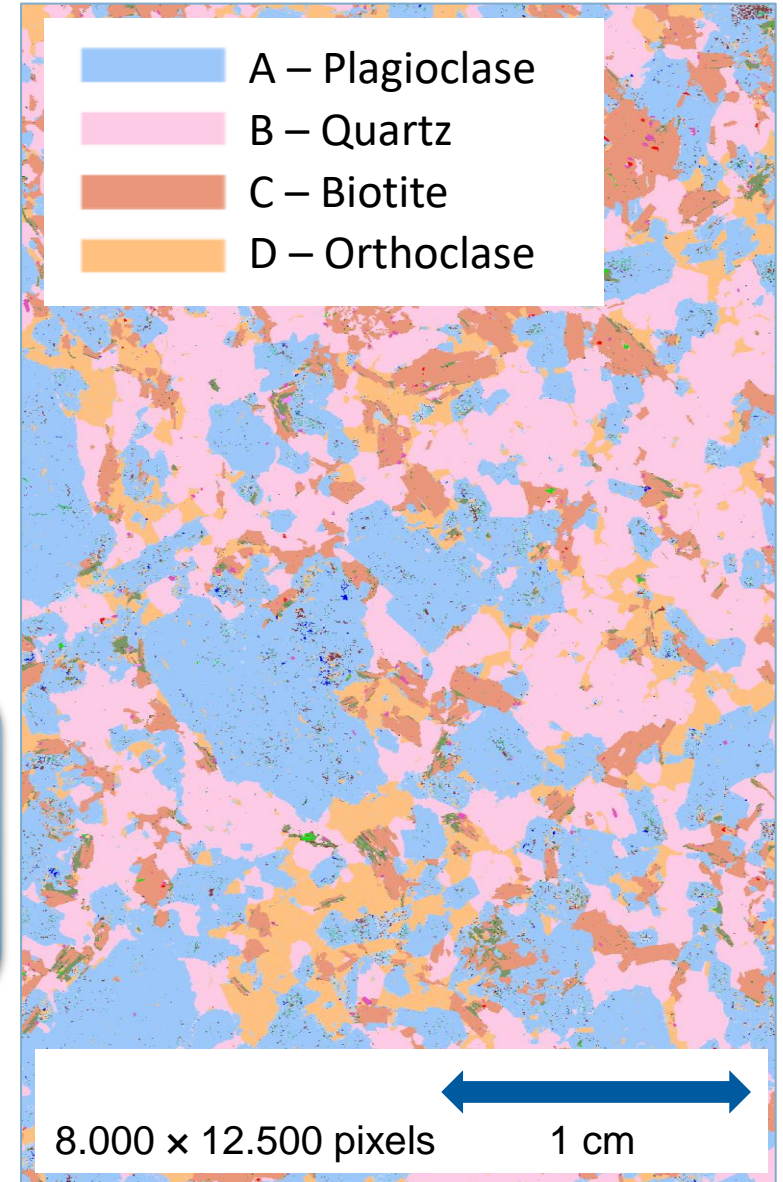
Determination of the optimum RVE

Check the preservation of the "statistics of the material"
via sliding area window

Relative number of pixels per category

MLA: Mineral Liberation Analysis - Measurements and postprocessing
performed by Kai Bachmann (Helmholtz Institute Freiberg for
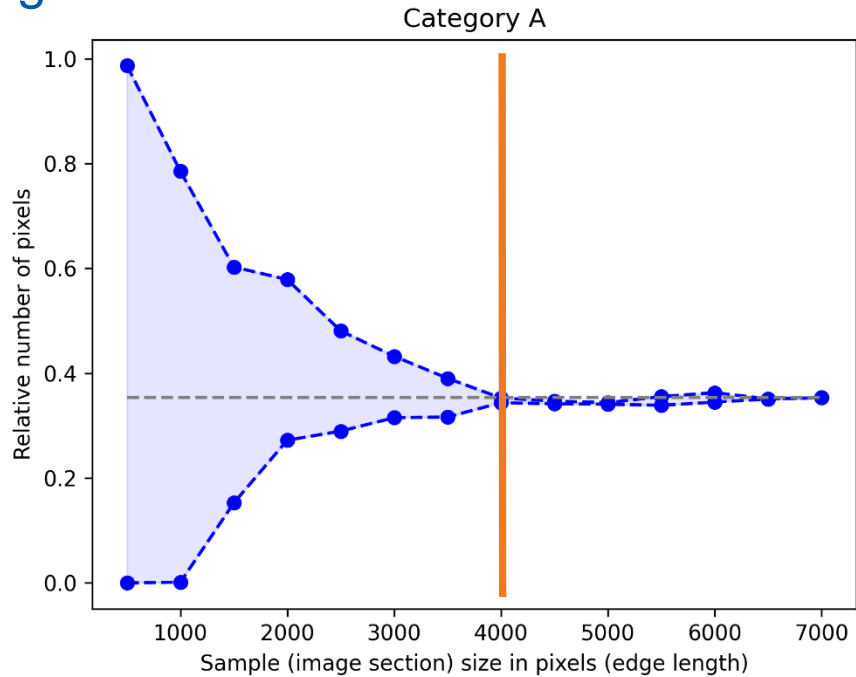Resource Technology, Department Electron Beam Analytics)

A – Plagioclase
B – Quartz
C – Biotite
D – Orthoclase

Training data:
MLA samples
from Germany's
Lusatia region

8.000 × 12.500 pixels   1 cm

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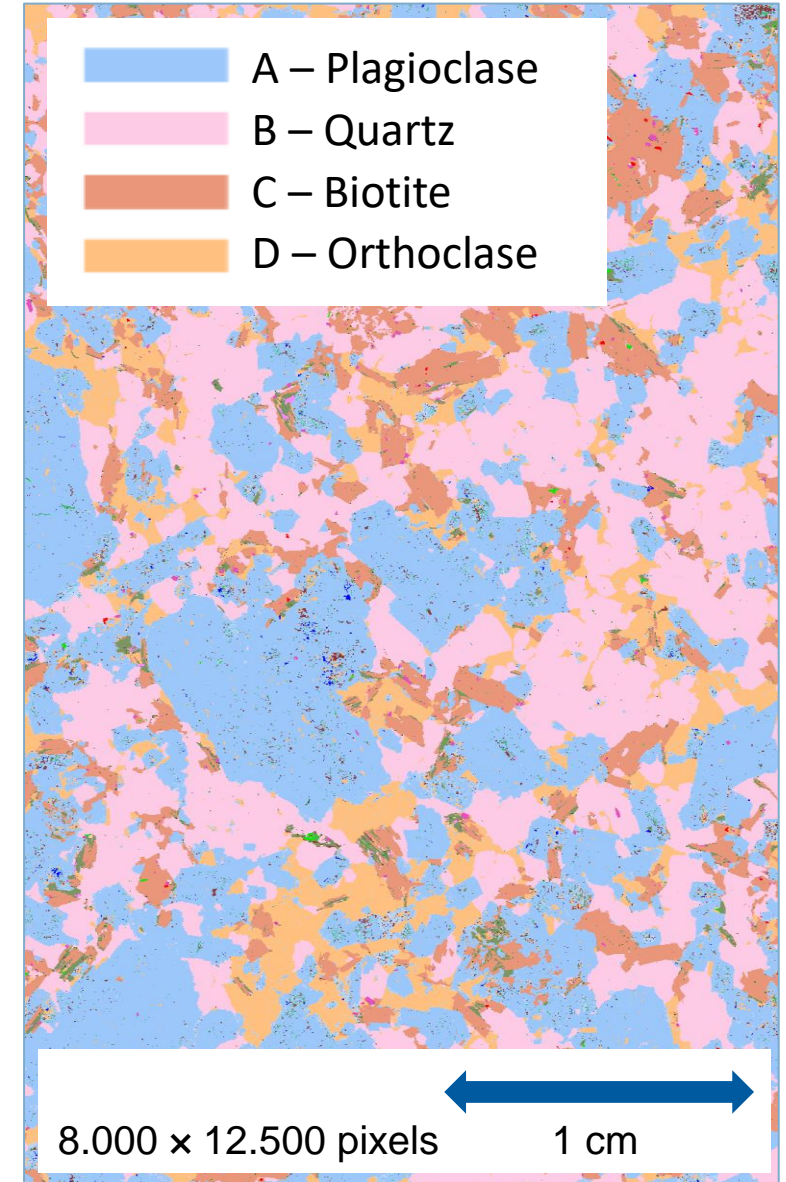Clausthal University of Technology   SCIENCE AND INNOVATION CAMPUS

Determination of the optimum RVE

Check the preservation of the "statistics of the material" via sliding window

At what RVE size does a certain category have the same relative frequency as in the overall sample?

A – Plagioclase
B – Quartz
C – Biotite
D – Orthoclase

8.000 × 12.500 pixels   1 cm

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Determination of the optimum RVE

Check the preservation of the "statistics of the material"
via sliding window

A – Plagioclase
B – Quartz
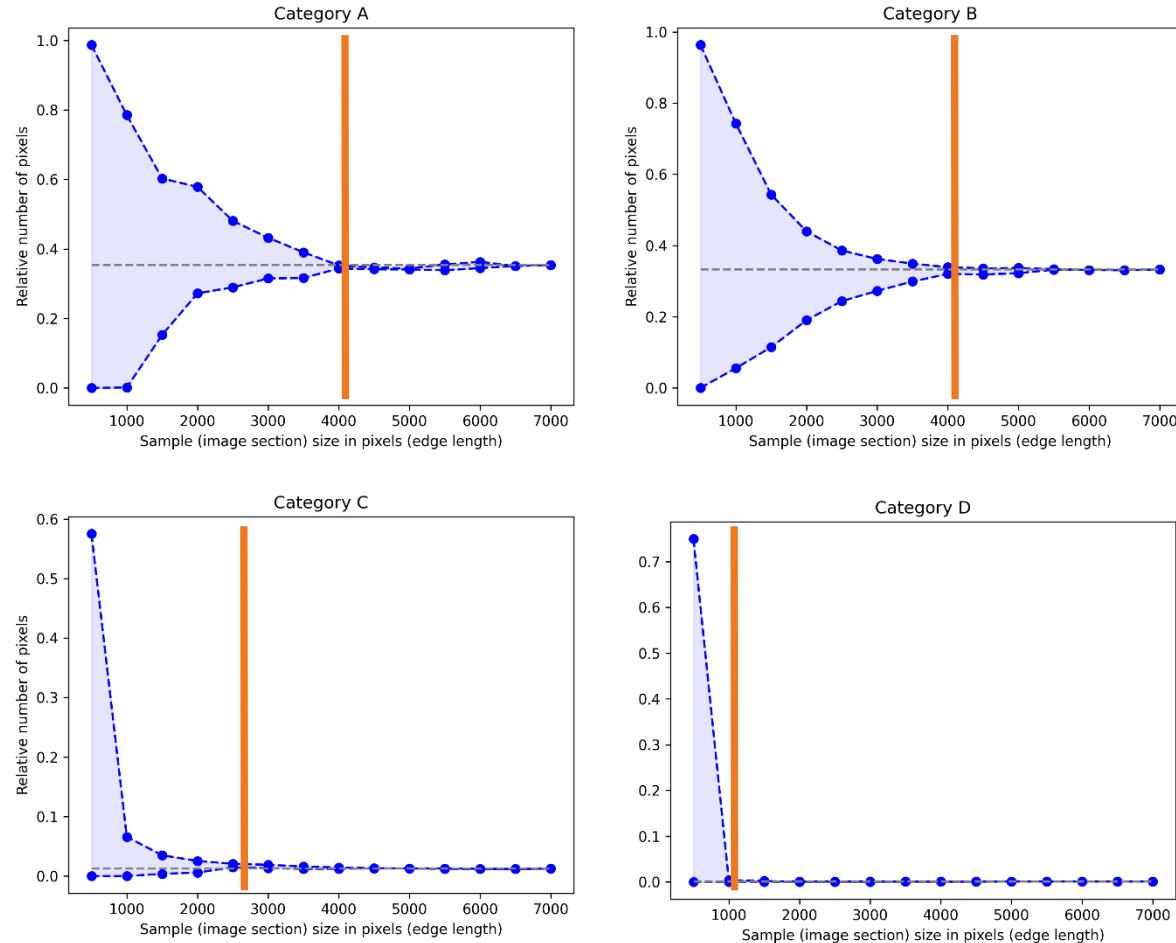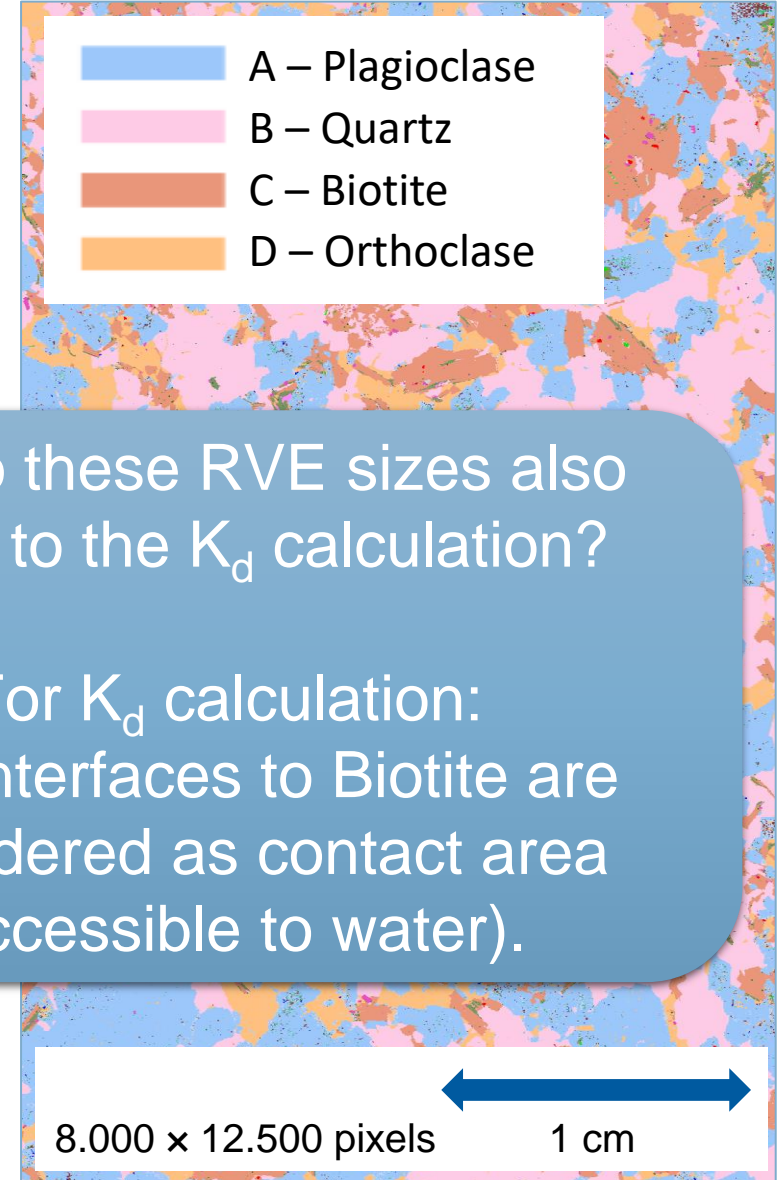C – Biotite
D – Orthoclase

But do these RVE sizes also apply to the K_d calculation?

For K_d calculation:
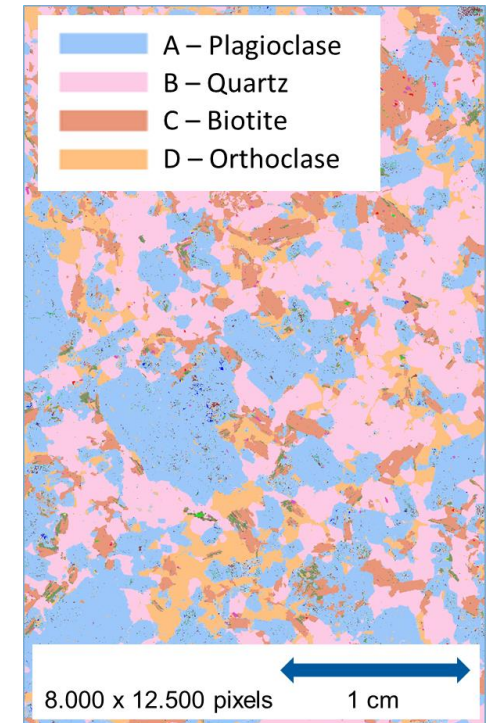only interfaces to Biotite are considered as contact area (accessible to water).

8.000 × 12.500 pixels   1 cm

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Determination of the optimum RVE

Variogram calculation

Training data: MLA samples from Lusatia

- Implementation in Python using GSTools API
- Gaussian processes with Matérn covariance function

Müller, S., Schüler, L., Zech, A., and Heße, F.: GSTools v1.3: a toolbox for geostatistical modelling in Python, Geosci. Model Dev., 15, 3161–3182, https://doi.org/10.5194/gmd-15-3161-2022, 2022.

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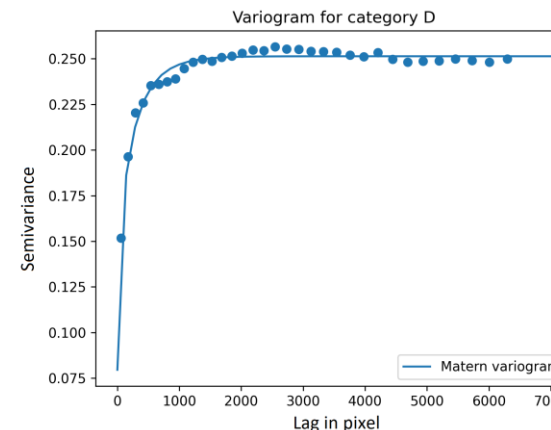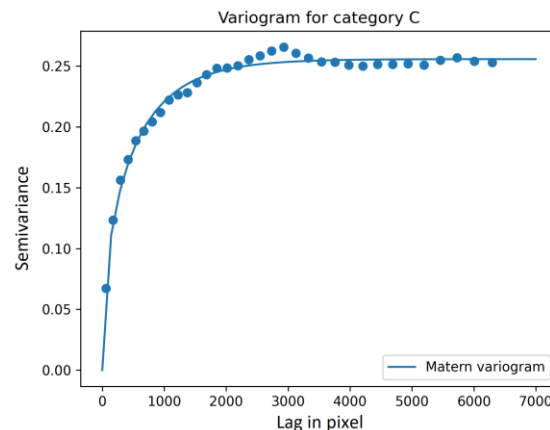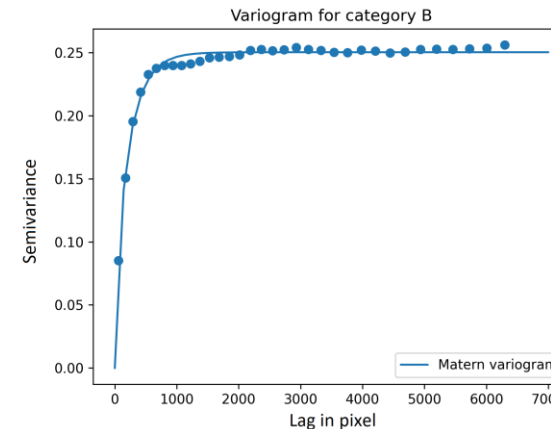
Determination of the optimum RVE

Variogram calculation

Training data: MLA samples from Lusatia

Simulation of the crystalline rock

RVE sizes between 500✕500 and 6500✕6500 pixels - 20 simulations each

A – Plagioclase
B – Quartz
C – Biotite
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8.000 x 12.500 pixels   1 cm

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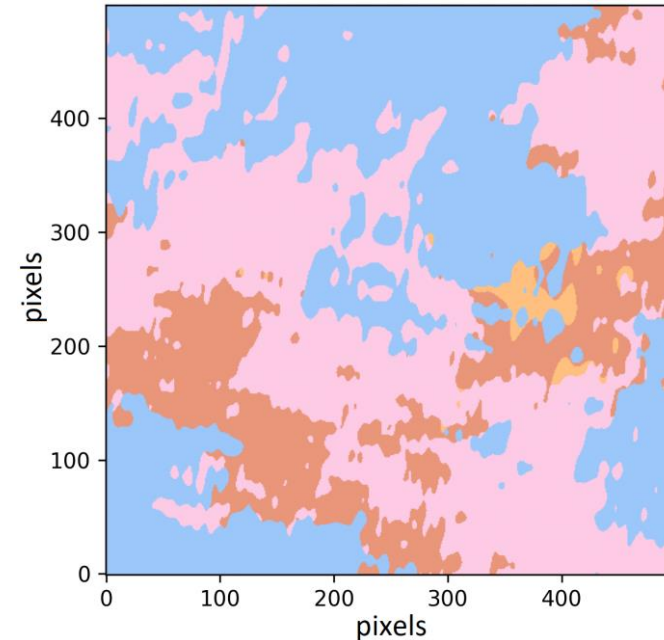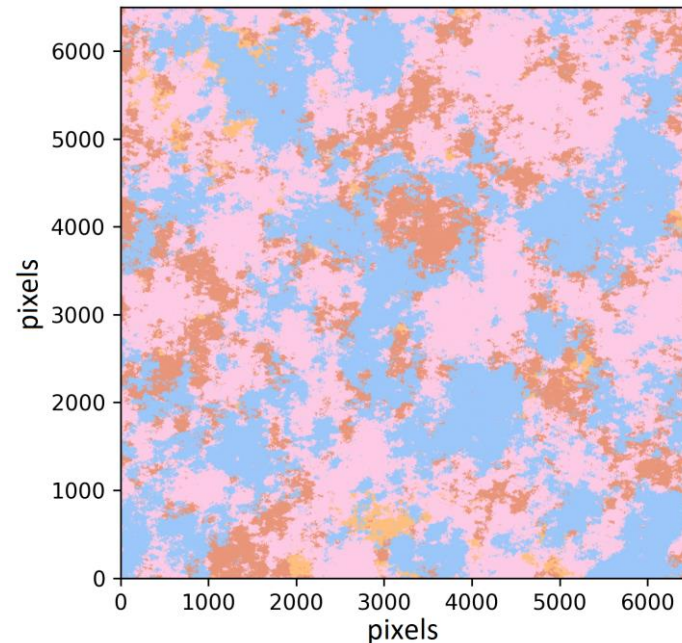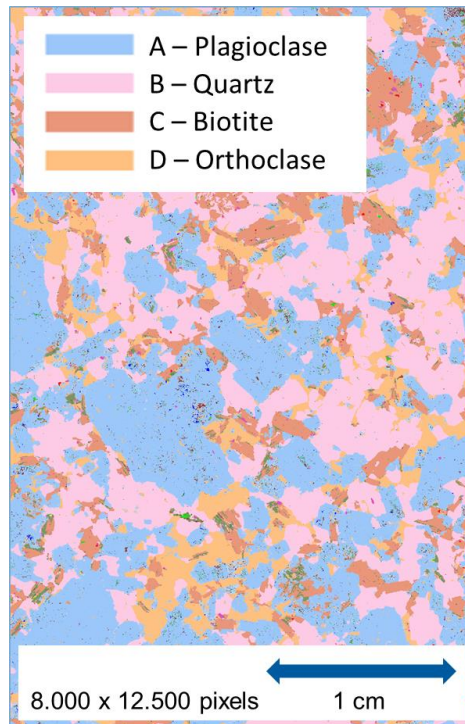
Determination of the optimum RVE

Variogram calculation

Training data: MLA samples from Lusatia

Simulation of the crystalline rock

RVE sizes between 500✕500 and 6500✕6500 pixels - 20 simulations each

Parameterization of the model

Mineral & groundwater composition, thermodynamic sorption data

pH	8.74
Eh	100 mV
Ratio rock/fluid	25
UO_2^{++}	$0.5 \cdot 10^{-3}$ mol/l

Na^+	$5.2 \cdot 10^{-3}$ mol/l	F^-	$8.2 \cdot 10^{-5}$ mol/l
K^+	$2.4 \cdot 10^{-5}$ mol/l	SO_4^{--}	$1.4 \cdot 10^{-3}$ mol/l
Mg^{++}	$1.6 \cdot 10^{-6}$ mol/l	HCO_3^-	$1.8 \cdot 10^{-3}$ mol/l
Ca^{++}	$3.0 \cdot 10^{-4}$ mol/l	Al^{+++}	$1.0 \cdot 10^{-10}$ mol/l
Cl^-	$2.7 \cdot 10^{-3}$ mol/l	$Si(OH)_4$	$1.0 \cdot 10^{-10}$ mol/l
NO_3^-	$1.6 \cdot 10^{-6}$ mol/l	Fe^{+++}	$1.0 \cdot 10^{-10}$ mol/l

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Determination of the optimum RVE

Variogram calculation

Training data: MLA samples from Lusatia

Simulation of the crystalline rock

RVE sizes between 500✕500 and 6500✕6500 pixels - 20 simulations each

Parameterization of the model

Mineral & groundwater composition, thermodynamic sorption data

Geochemical reaction simulation
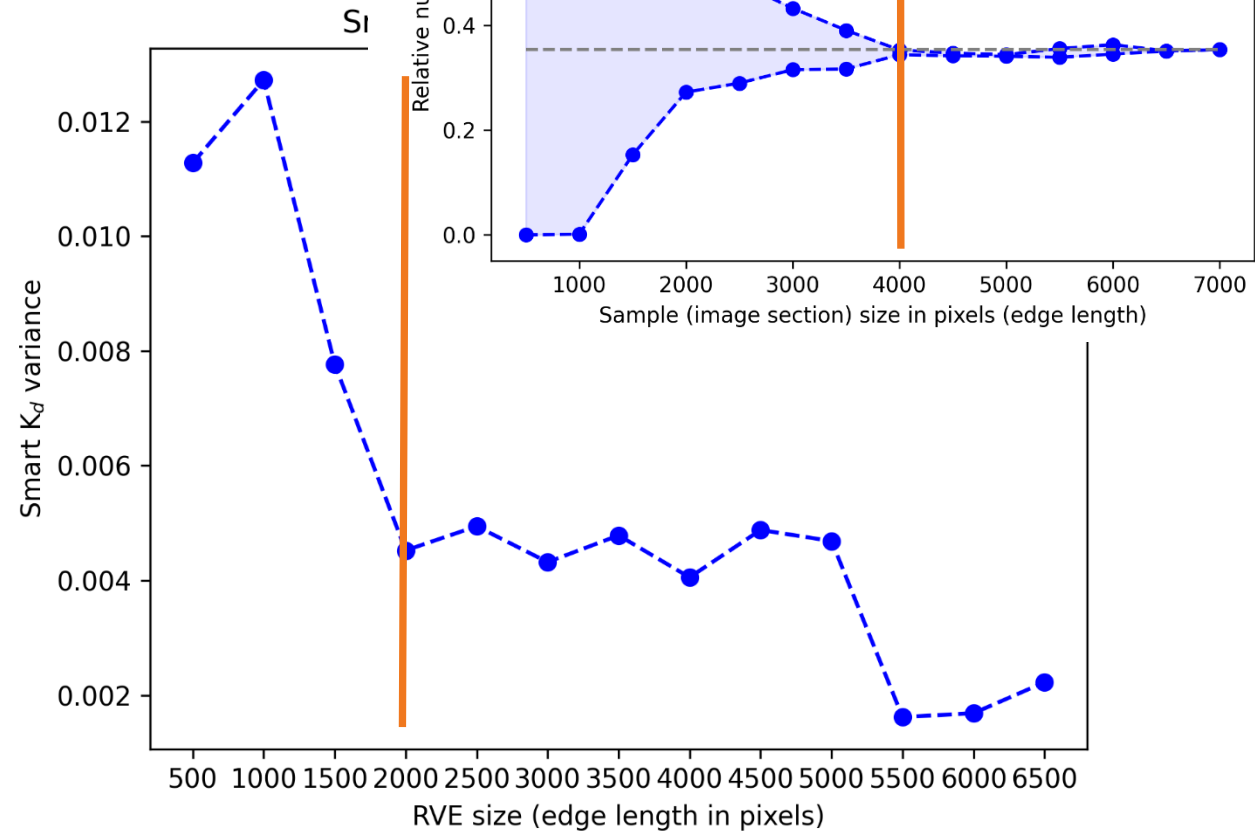
Smart K_d calculation for Uranium

Determination of the optimum RVE

Smallest K_d variance

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Determination of the optimum RVE

Smart K_d calculation for Uranium → Smallest K_d variance

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Take home message

- For a **rough approximation** the size of the optimal RVE can be estimated by checking the statistical preservation – even in the case of the Kd calculation

- Advantage of variogram calculation and simulation: method considers **variations in grain size and grain distribution**

Thank you for your attention!

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Understanding Geological Key Factors for Radionuclide Retention: Insights from Sensitivity Analysis on Varied Crystalline Host Rock Compositions ▶

Solveig Pospiech, Frank Bok, Mostafa Abdelhafiz, Alexandra Duckstein, Elmar Plischke, and Vinzenz Brendler

Tue, 16 Apr, 16:15–18:00 (CEST)

Hall X4 | X4.145

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