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3-D stochastic geological modelling of the sediment texture in detrital systems: prediction of fictive grain size distributions and uncertainty quantification

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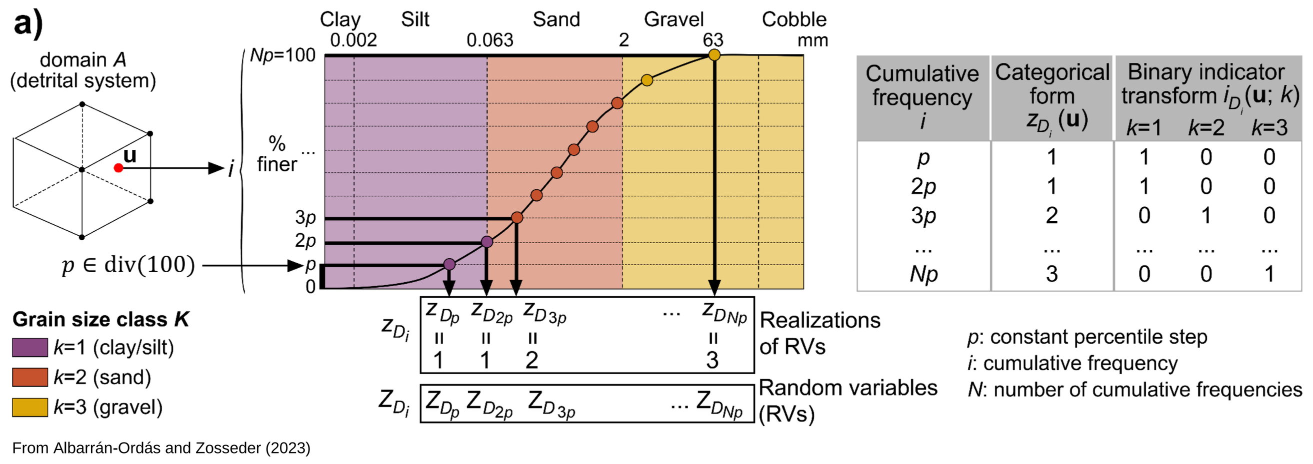
INTRODUCTION

Geological 3-D modelling of the grain size distribution (GSD): the D_i models method

The D_i models method mimics the GSD characterization at each cumulative frequency in the random function space



From Albarrán-Ordás and Zosseder (2023)

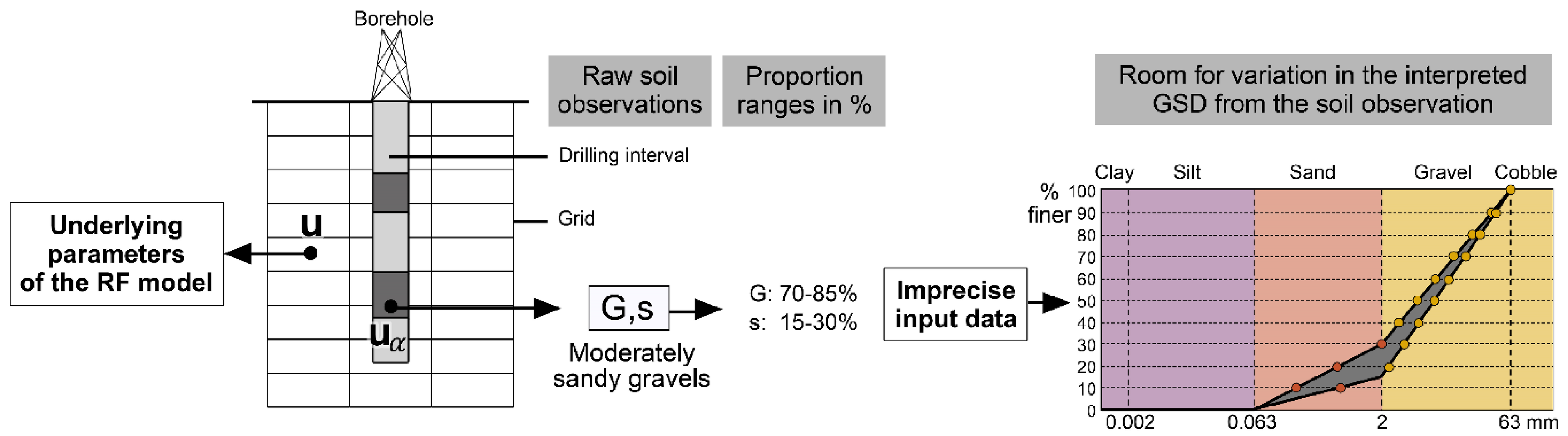
Random Function Space

Definition of a **rule for each D_i** that assigns a collection of alternative realities (set of realizations) **that replaces the unknown reality** and shares with it:
- statistics and
- patterns of spatial continuity

for each D_i

Uncertainties in the context of the D_i models method

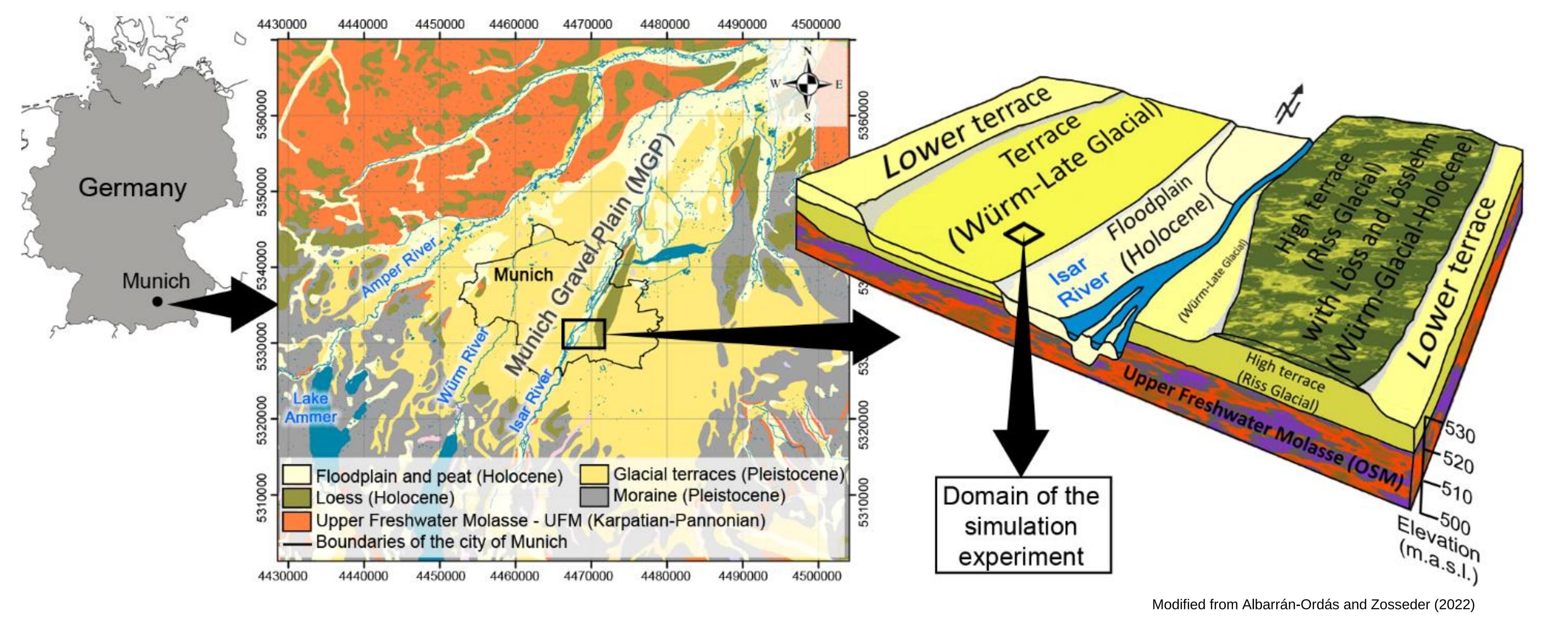
- Uncertainties are linked to the developed **Random Function (RF) model**: RVs, (non)-stationarity decisions
- **Imprecise input data**: direct soil observations from drilled materials described in the field are subjected to natural geological variability and systematic imprecisions associated with the inherent generalizations of the standards used and to the subjectivity of on-site personnel



Research goals

1. Adapting the framework of the D_i models method to **integrate uncertainties from imprecise input data**
2. Developing **uncertainty quantification (UQ) measures** linked to: a) each D_i, and b) the whole mixture of clasts
3. Evaluating the ability of the UQ measures **with different RF models**
4. Exploring the **uncertainty propagation and impacts** of the adaptation of the geostatistical framework

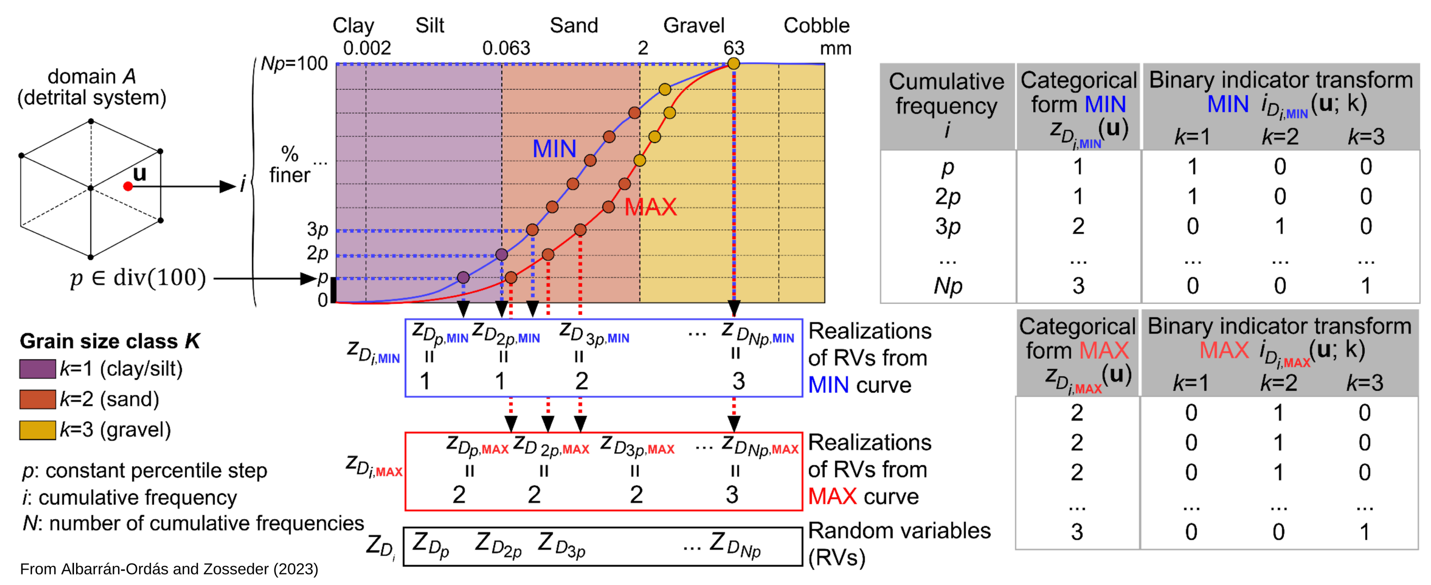
Geological setting for the simulation experiment



Modified from Albarrán-Ordás and Zosseder (2022)

MATERIAL AND METHODS

Adapting the geostatistical framework of the D_i models method to integrate uncertainties from imprecise input data



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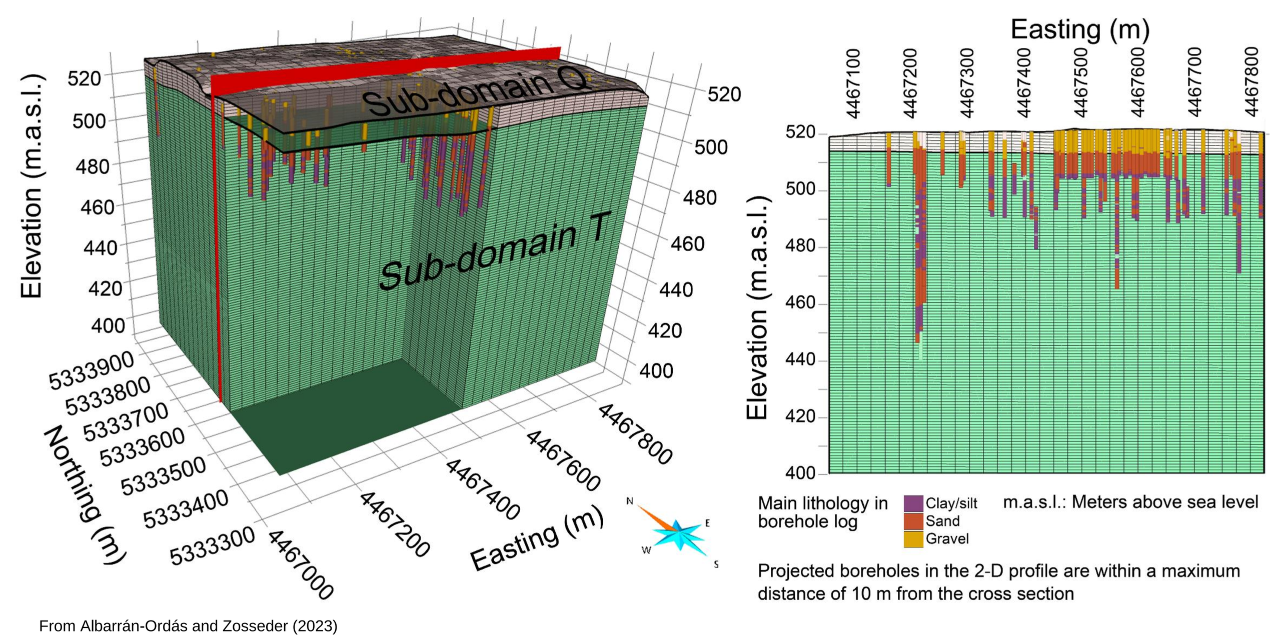
Simulation experiment: domain and conceptual model



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- Dimensions: 765 x 580 x 133 m
- Cell size: 25 x 25 x 1 m
- Input data: Direct soil observations from 416 boreholes
- Sub-domains: Q (Quaternary) T (Miocene, Tertiary)
- Grain size classes: k=1 (clay/silt), k=2 (sand), k=3 (gravel)
- Constant step in the GSD: p=10

Simulation experiment: setups with (non)-stationarity assumptions

Setup	Domain	Indicator kriging algorithm	3-D trend model	Adapted geo-modeling framework
1	Entire	Stationary SK	No	Yes
2	Q and T	Stationary SK	No	Yes
3	Q and T	Non-stationary SK (LVM)	Yes, highly overfit	Yes
4	Q and T	Non-stationary SK (LVM)	Yes, slightly overfit	Yes
5	Q and T	Non-stationary SK (LVM)	Yes, non-overfit	Yes
6	Q and T	Non-stationary SK (LVM)	Same as 5 but only MIN trends	No, finest-grained
7	Q and T	Non-stationary SK (LVM)	Same as 5 but only MAX trends	No, coarsest-grained

Uncertainty quantification (UQ) measures

- **Uncertainty for each D_i** in terms of the entropy of the discrete distribution

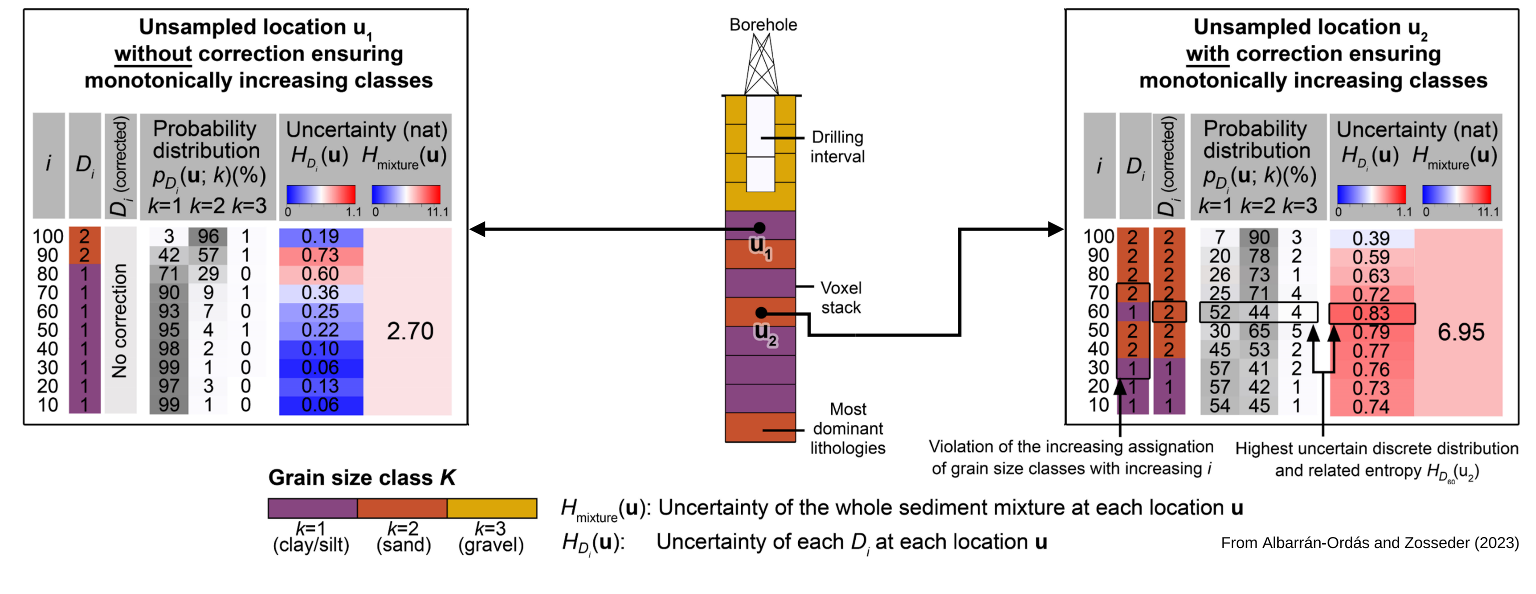
$$H_{D_i}(\mathbf{u}) = -\sum_{k=1}^{K} p_{D_i}(\mathbf{u};k)\ln\left[p_{D_i}(\mathbf{u};k)\right]; \quad k=1,\dots,K;\ \mathbf{u}\in A$$

- **Uncertainty about the whole sediment mixture** as a combined system formed by a collection of RVs:

$$H_{\text{mixture}}(\mathbf{u}) = H\left[Z_{D_{100}}(\mathbf{u}), Z_{D_{100-p}}(\mathbf{u}), \dots, Z_{D_p}(\mathbf{u})\right] = H\left[Z_{D_{100}}(\mathbf{u})\right] + H\left[Z_{D_{100-p}}(\mathbf{u})\right] + \dots + H\left[Z_{D_p}(\mathbf{u})\right]$$

RESULTS AND CONCLUSIONS

Entropy-based correction for ensuring monotonically increasing GSD



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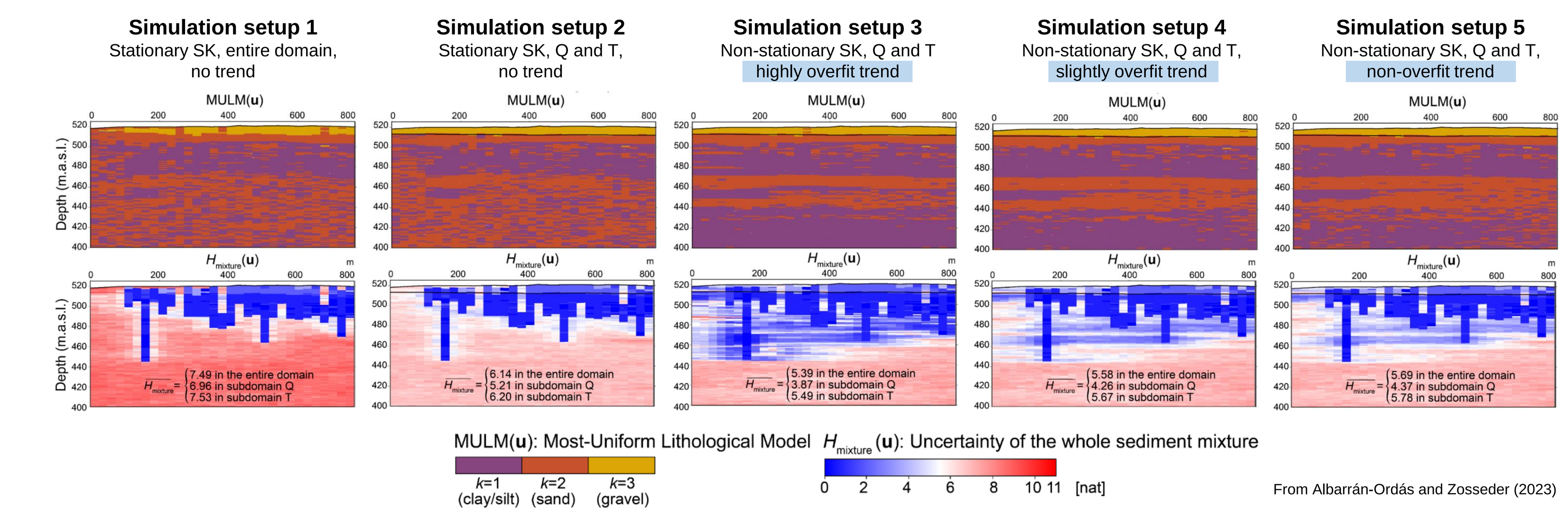
Uncertainty quantification (UQ) in the whole sediment mixture

- **UQ measures**: useful for **quantifying** and **comparing** uncertainties, **scalable** with other conceptual models
- Simulating the **entire domain** leads to a lack of representativeness of spatial statistics: poor estimation (setup 1)
- Simulating the **sub-domains** (from setup 2) and including **3-D trends** (3, 4, 5) improve the estimation
- Trend overfitting leads to overestimation and unfair uncertainties (3, 4). Trend modeling/evaluation: key and critical



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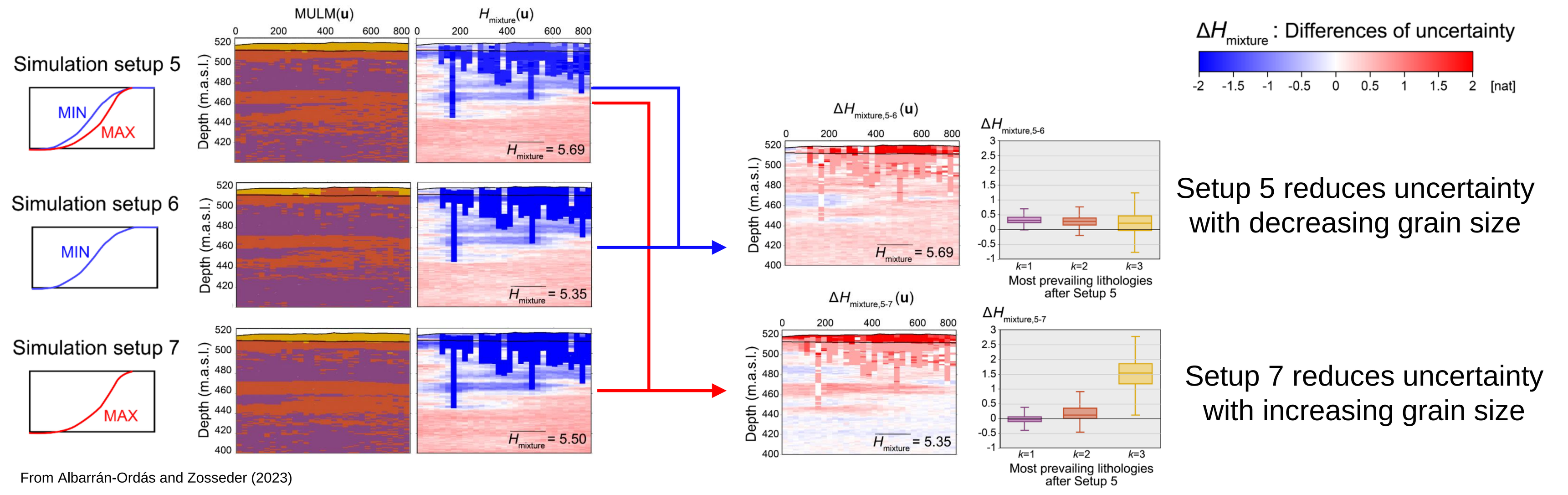
Impacts of adapting the geostatistical framework on the uncertainty propagation

- More realistic uncertainty assessment by overcoming the bias caused by ignoring imprecise input data (represented by two extreme unique interpretations of the GSD: MIN, MAX)



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Conclusions

- Imprecisions in soil observations from boreholes are integrated into 3D geo-modelling
- Entropy-based measures quantify the uncertainty of the grain size range of the soil
- A more realistic uncertainty assessment is provided due to overcome potential bias
- Better understanding of parameters of the random functions in the D_i models method
- The uncertainty scheme supports the decision-making process for practical purposes

REFERENCES

- Albarrán-Ordás, A., Zosseder, K (2022). The Di models method: geological 3-D modeling of detrital systems consisting of varying grain fractions to predict the relative lithological variability for a multipurpose usability. Bulletin of Engineering Geology and the Environment 81:34. DOI: 10.1127/zdgg/2020/0206
- Albarrán-Ordás, A., Zosseder, K (2023). Uncertainties in 3-D stochastic geological modelling of fictive grain size distributions in detrital systems [Manuscript submitted for publication]

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