A Spatial-Autocorrelation Workflow for Data-Driven Confidence Mapping of Geological Surfaces

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GSEU Workshop: Exploring, Quantifying and Communicating Uncertainties in Geological Models – March 2-3, 2026

Introduction

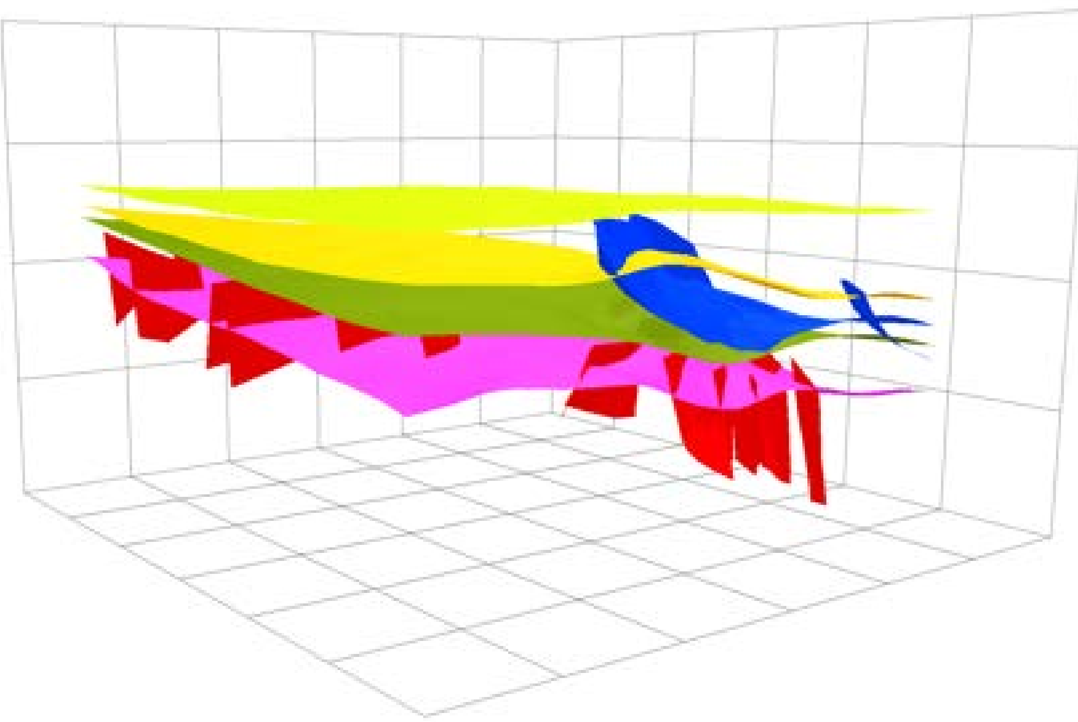
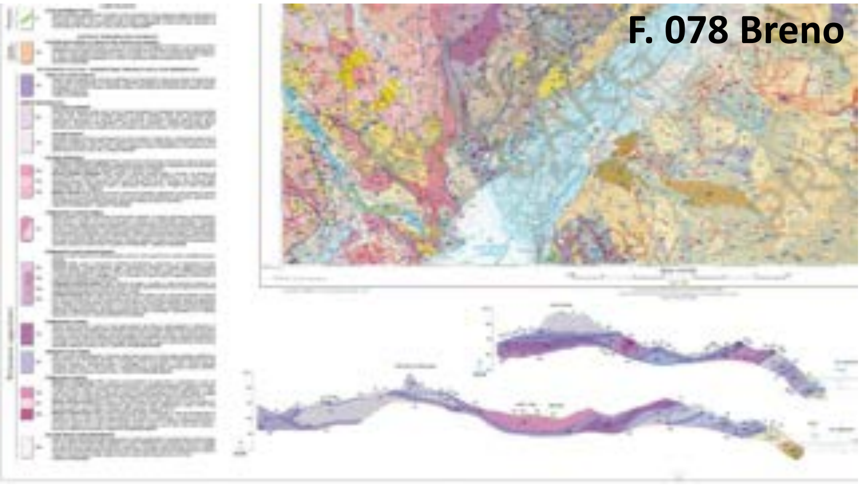


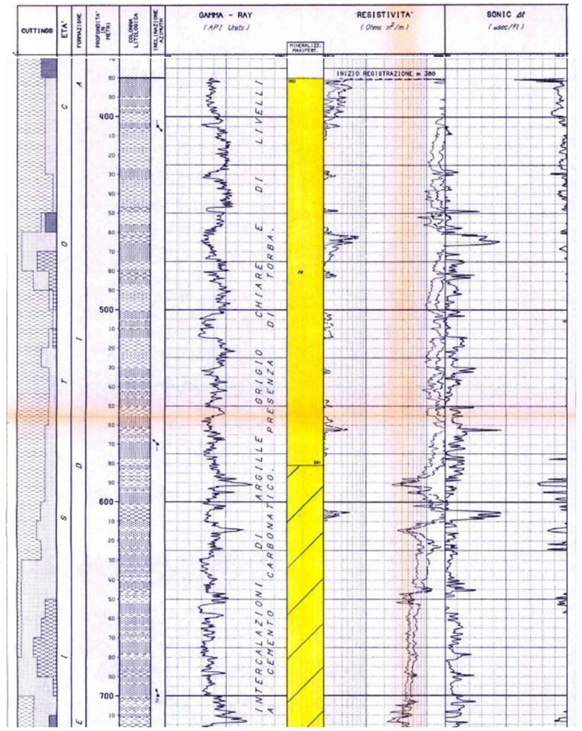
Image from GEO-IT3D Geological 3D models in Italy

3D web-viewer

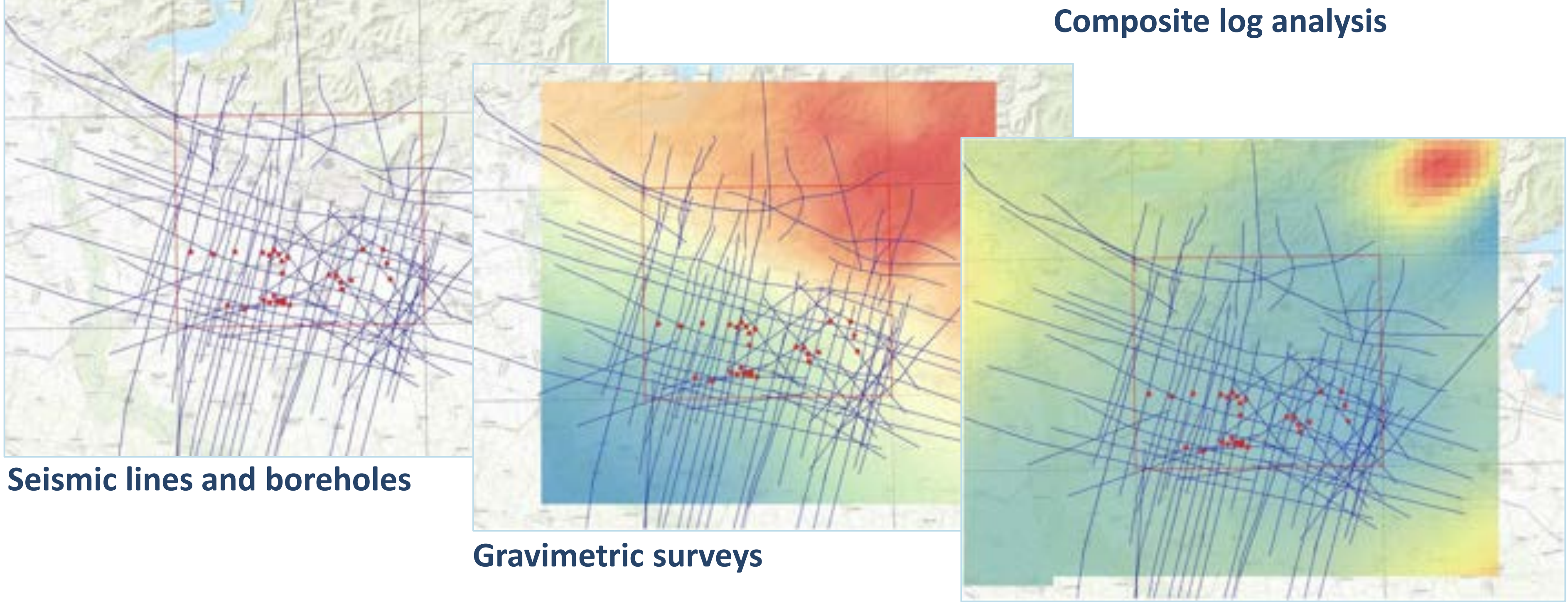
https://geo-it3d.isprambiente.it/map



Geological survey



Composite log analysis



Seismic lines and boreholes

Gravimetric surveys

Aeromagnetic surveys

State of The Art

«**Quality flagging** is the basic approach used to quantify uncertainty within a spatial dataset and is done by assessing metadata fields; This approach may range from simply indicating data presence or absence to more complex methods yielding a comprehensive array of quantitative error ranges»

QJEGH

Research article

Quarterly Journal of Engineering Geology and Hydrogeology

https://doi.org/10.1144/qjegh2020-028 | Vol. 54 | 2020 | qjegh2020-028

Uncertainty assessment applied to marine subsurface datasets

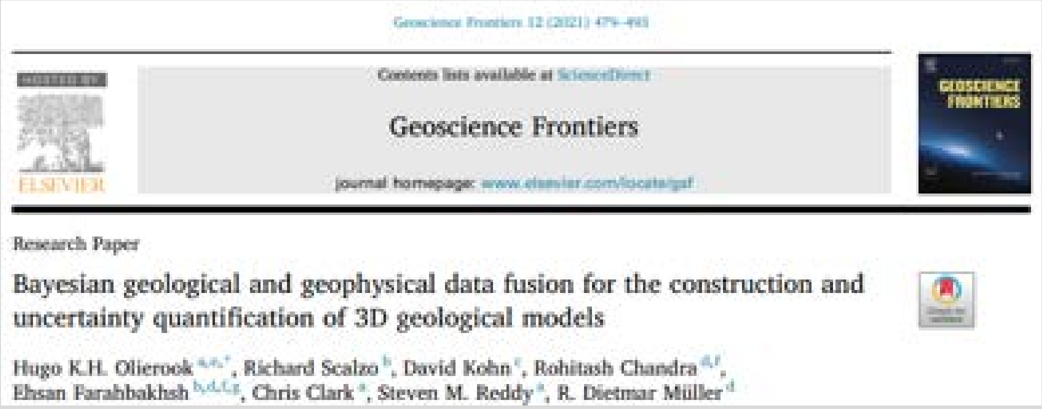
Lars Kint[1*], Vasilis Hademenos[2], Robin De Mol[3], Jan Stafleu[4], Sytze van Heteren[4] and Vera Van Lancker[1,2]

Natural Resources Research, Vol. 10, No. 3, September 2001 (© 2001)

Traditional and New Ways to Handle Uncertainty in Geology

George Bárdossy[1] and János Fodor[2]

«**Probabilistic** and **Machine Learning models** are usually difficult to set up, computationally demanding as well as difficult to interpret for decision makers»



Geoscience Frontiers 12 (2021) 479–493

Contents lists available at ScienceDirect

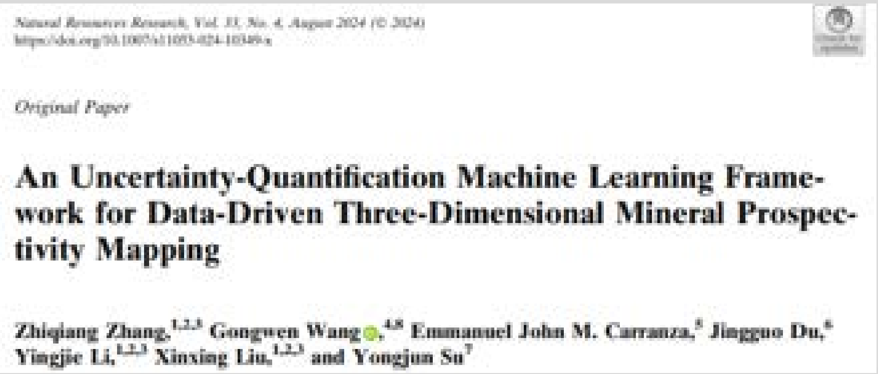
Geoscience Frontiers

journal homepage: www.elsevier.com/locate/gsf

Research Paper

Bayesian geological and geophysical data fusion for the construction and uncertainty quantification of 3D geological models

Hugo K.H. Olierook[a,e,*], Richard Scalzo[b], David Kohn[c], Rohitash Chandra[d,f], Ehsan Farahbakhsh[b,d,f,g], Chris Clark[a], Steven M. Reddy[a], R. Dietmar Müller[d]



Natural Resources Research, Vol. 33, No. 4, August 2024 (© 2024)
https://doi.org/10.1007/s11053-024-10349-x

Original Paper

An Uncertainty-Quantification Machine Learning Framework for Data-Driven Three-Dimensional Mineral Prospectivity Mapping

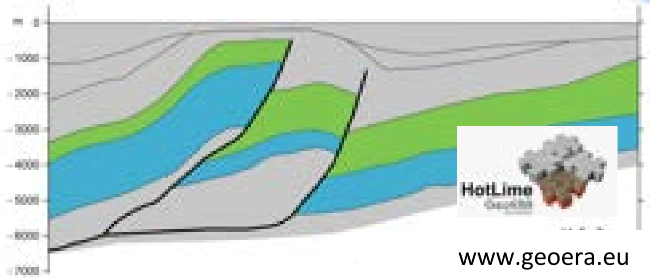
Zhiqiang Zhang,[1,2,3] Gongwen Wang,[4,8] Emmanuel John M. Carranza,[5] Jingguo Du,[6] Yingjie Li,[1,2,3] Xinxing Liu,[1,2,3] and Yongjun Su[7]

Limitations to a Generalized Approach for uncertainty

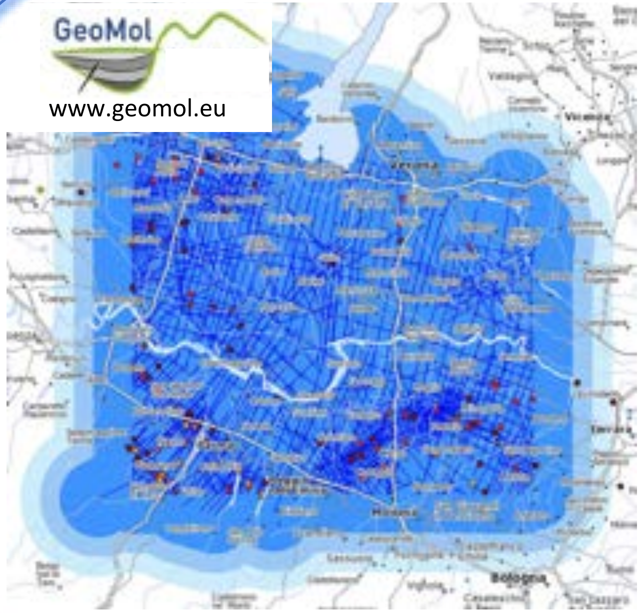
i) Areas with few constraining data
ii) Data with no attached uncertainty
iii) Inhomogeneous data availability and distribution
iv) No information about data acquisition techniques and instrumental accuracies
v) Errors on data models (e.g. Digital Terrain and Time/depths conversion models)
vi) Action Errors, Selection Errors, Information Retrieval Errors, Checking Errors (=Human errors)

Method

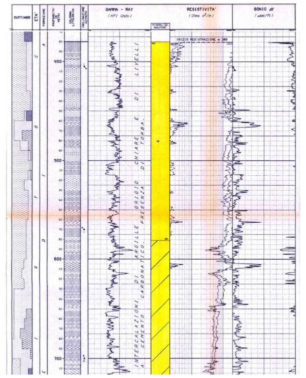
INPUT



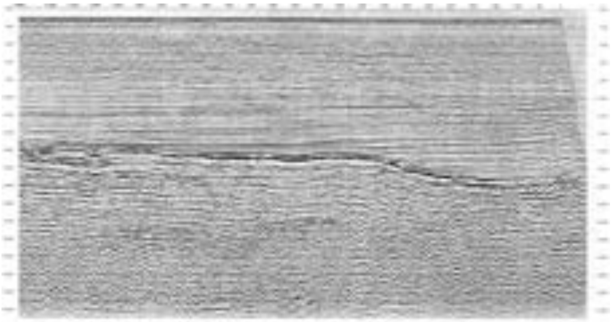
www.geoera.eu

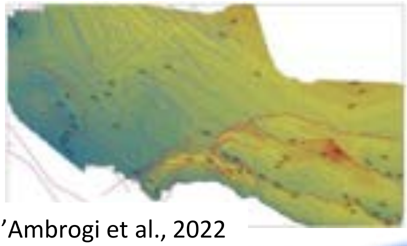


www.geomol.eu



ViDEPI





D'Ambrogi et al., 2022

What kind?

Types of Spatial Data
- punctual
- linear
- polygonal

How many?

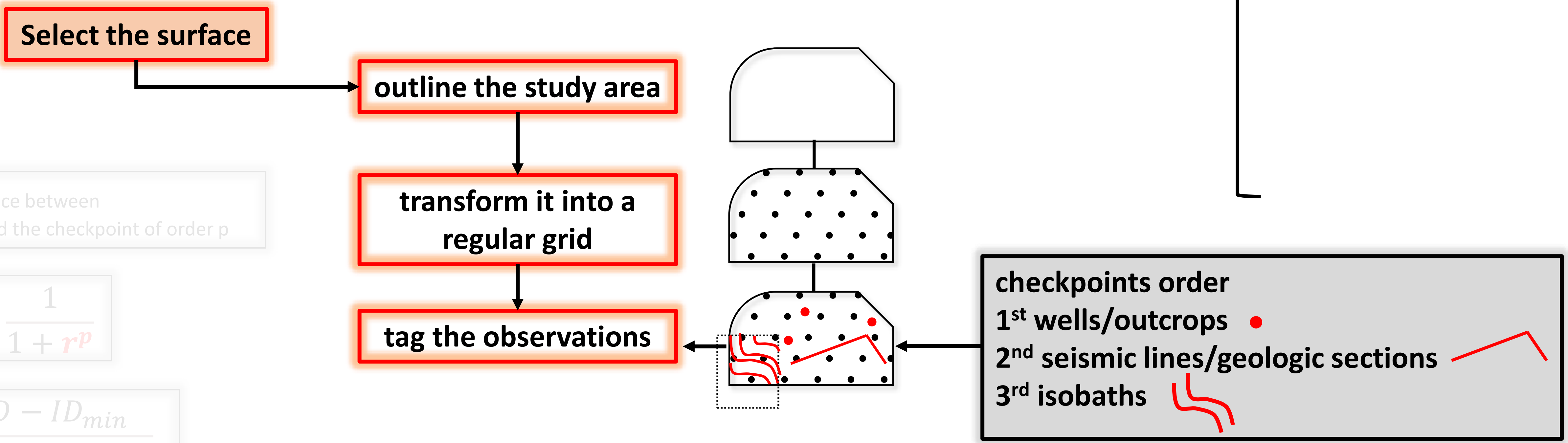
Count of Spatial Data
- n° punctual
- n° linear
- n° polygonal

How are they distributed?

Spatial autocorrelation measures the correlation between the values of a geographical variable as a function of the distance from the sampling points. **Key concept:** geographically close points tend to have similar values (positive autocorrelation).

Workflow

Pre-processing



Select the surface

outline the study area

transform it into a regular grid

tag the observations

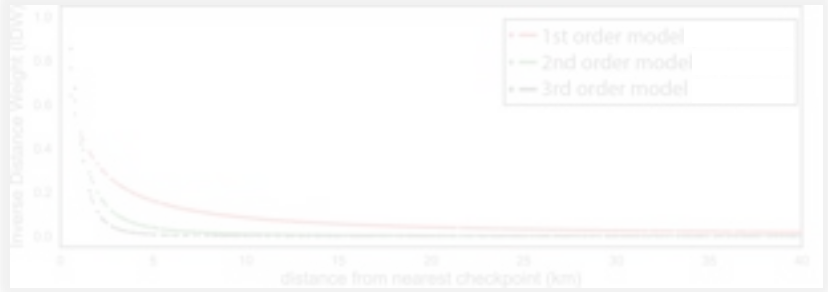
checkpoints order
1st wells/outcrops ●
2nd seismic lines/geologic sections
3rd isobaths

r^p = distance between the point of observation and the checkpoint of order p

$$IDW = \frac{1}{1 + r^p}$$

$$IDW_i = \frac{ID - ID_{min}}{ID_{MAX} - ID_{min}}$$

$$IDW_{avg} = \frac{1}{n}\sum_{i=1}^{p} IDW_i$$

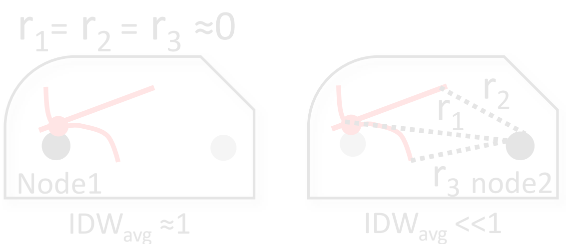


evaluate the horizontal confidence

evaluate the vertical confidence

interpolator (linear/NN)

$$\Delta_{norm} = 1 - \frac{\Delta - \Delta_{min}}{\Delta_{MAX} - \Delta_{min}}$$



collect matrices of confidence values

plot

Workflow

Pre-processing

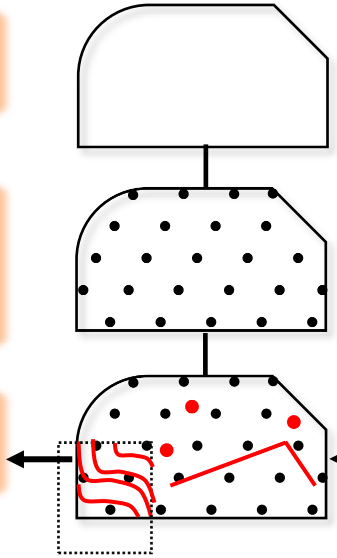
model

Select the surface

outline the study area

transform it into a regular grid

tag the observations



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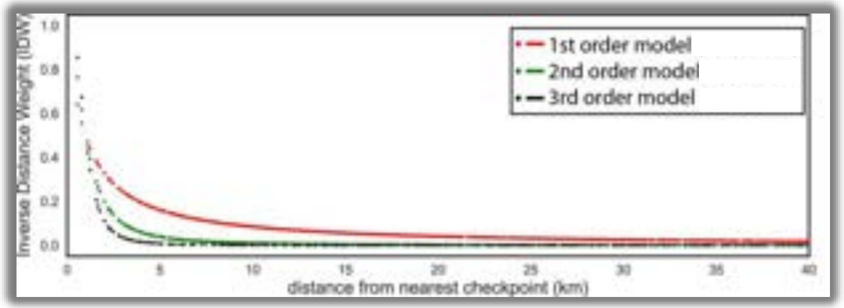

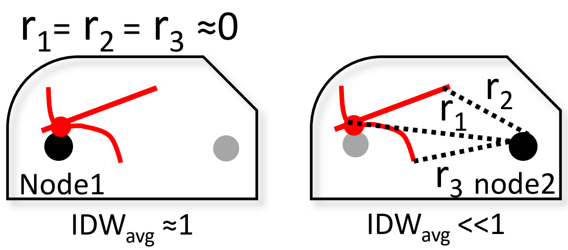

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Workflow

Pre-processing

model

processing

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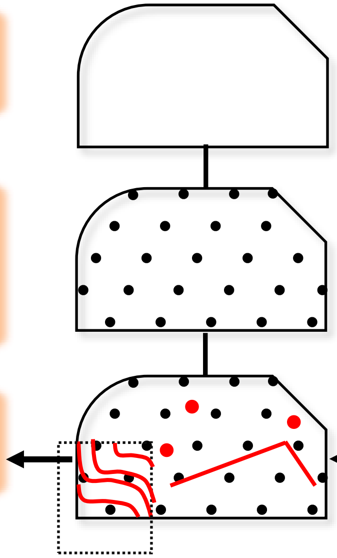

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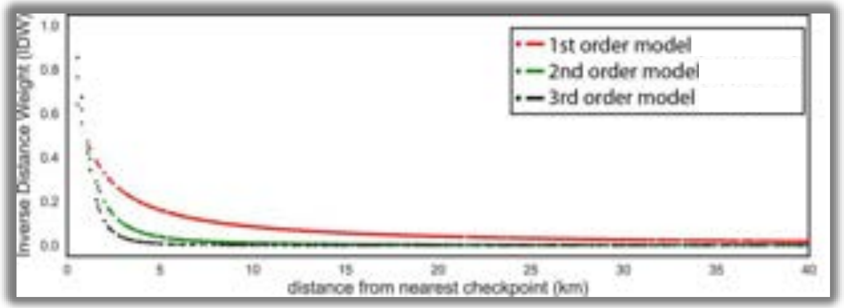
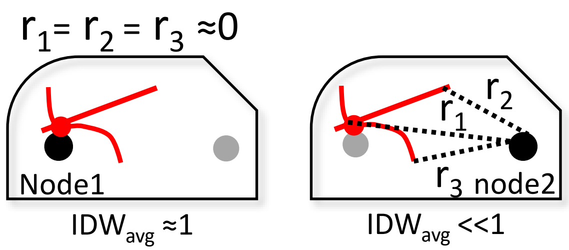
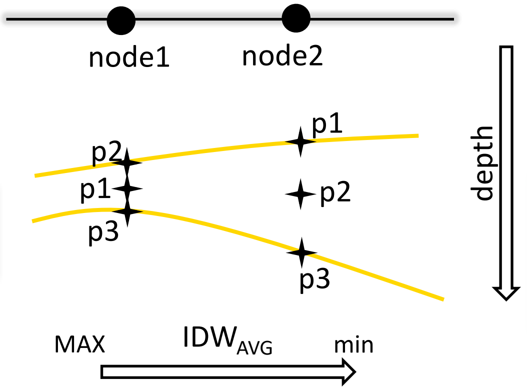


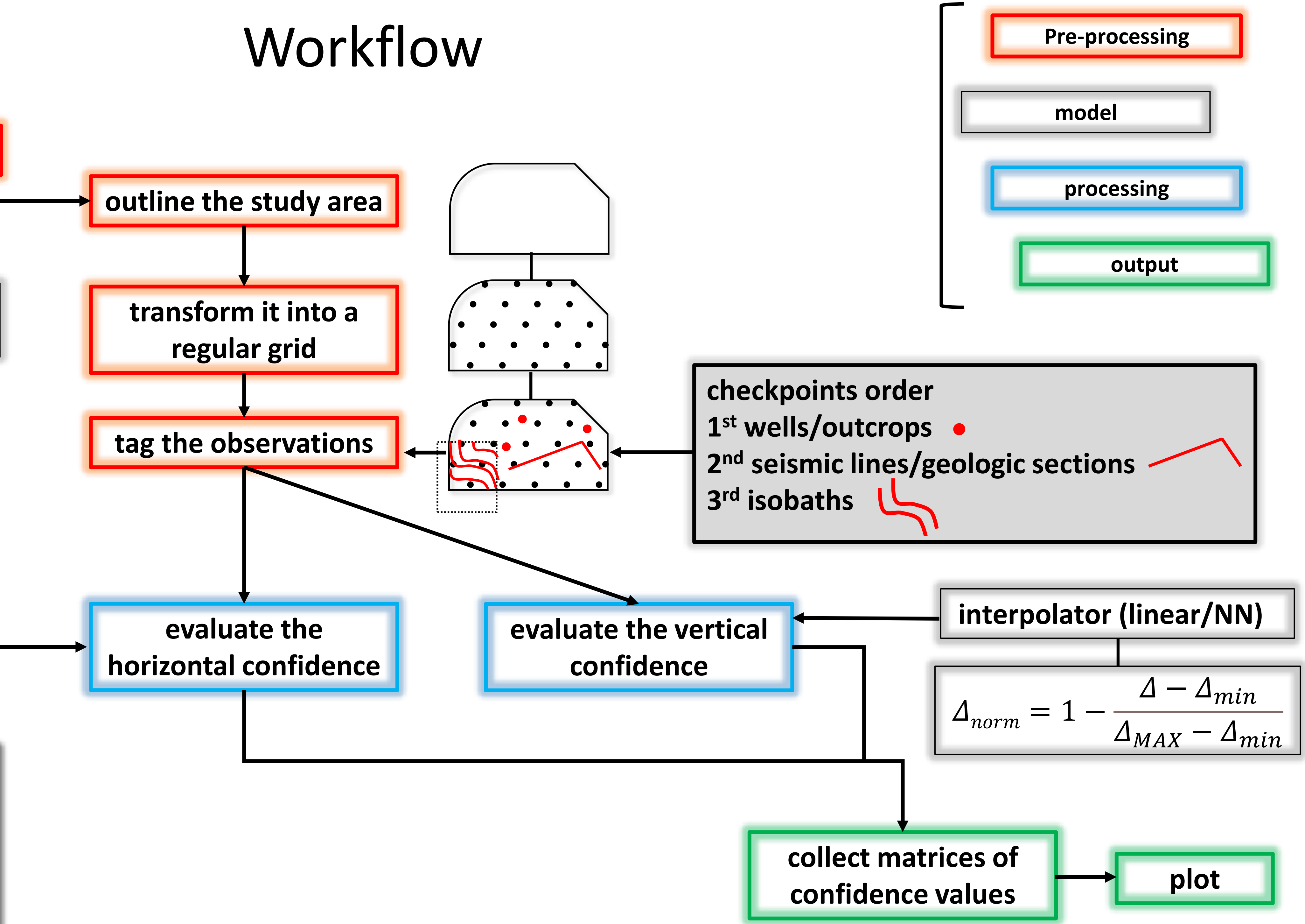




collect matrices of confidence values

plot

Workflow



Pre-processing

model

processing

output

Select the surface

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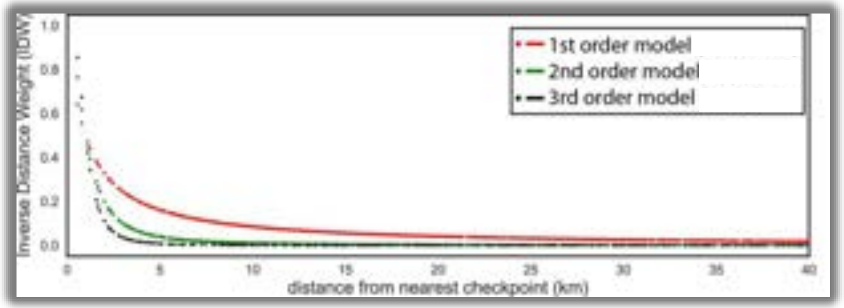
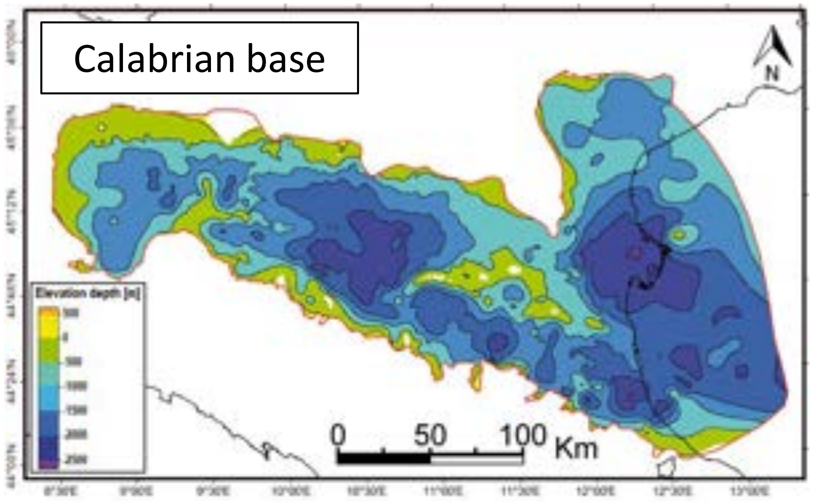
plot

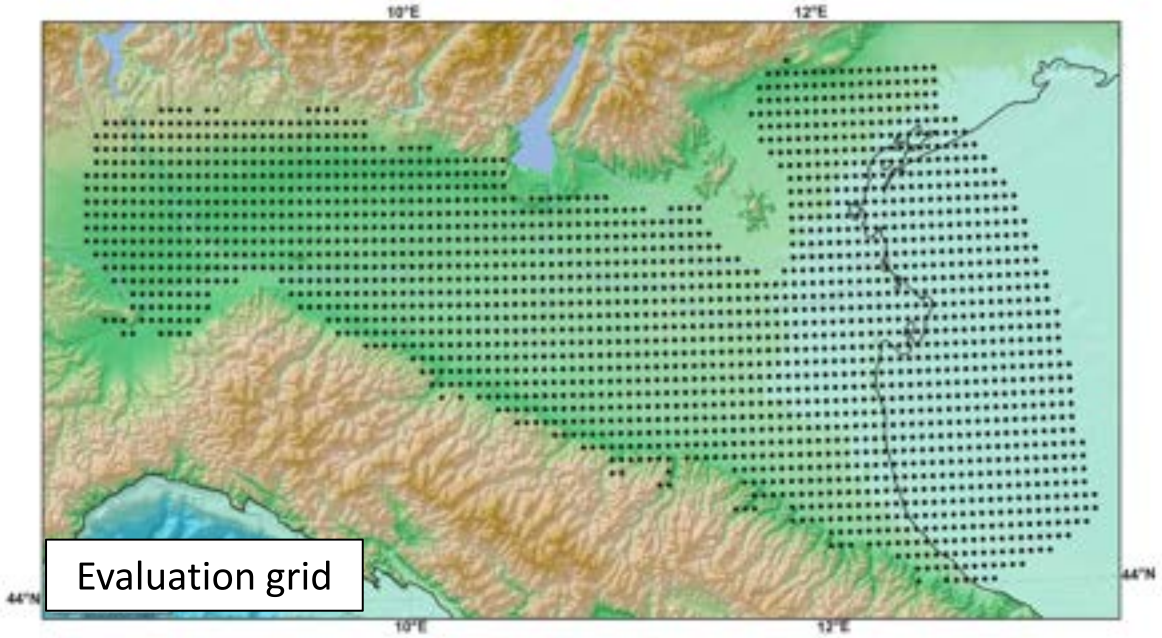


Example – evaluation grid

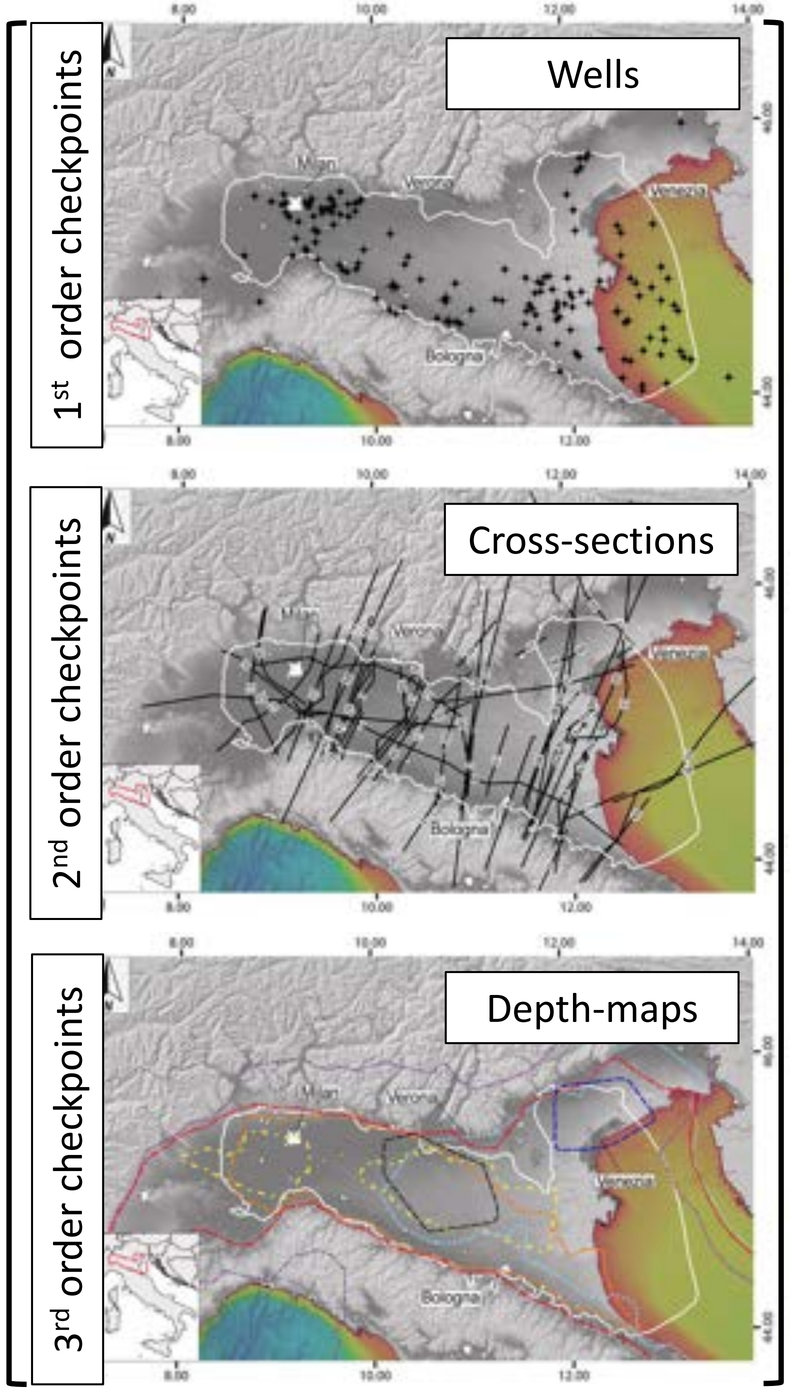
Pre-processing

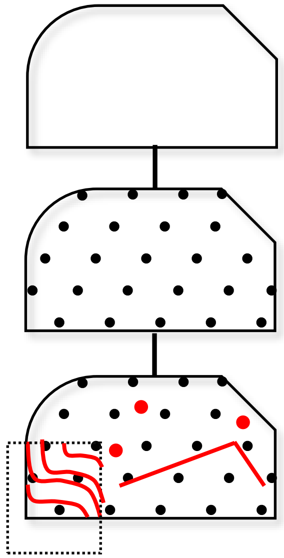


Livani et al., 2023

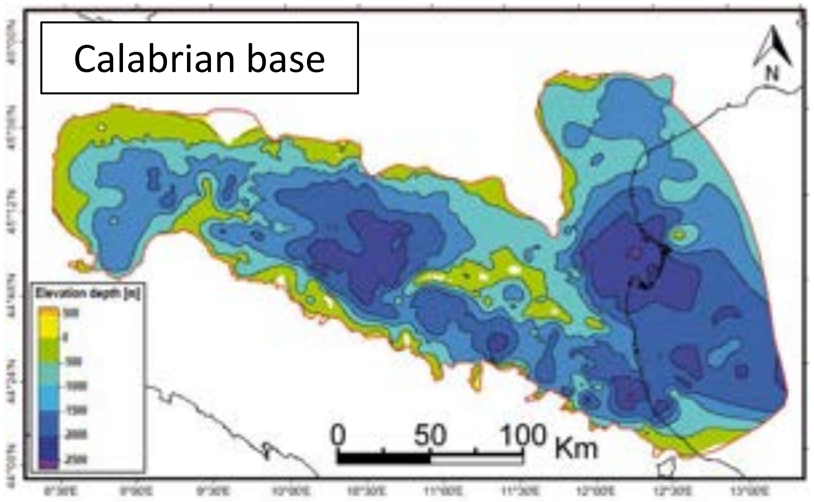


n. Checkpoint (p1)	n. Checkpoint (p2)	n. Checkpoint (p3)	Checkpoint density
139	3065	2299	2.36 per node

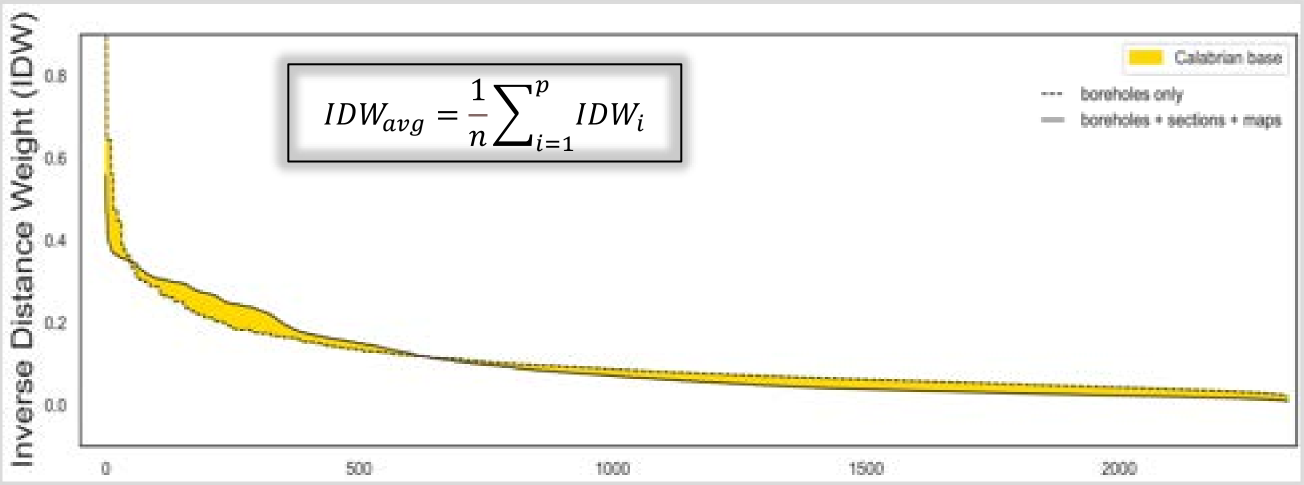




Example – horizontal accuracy



Livani et al., 2023



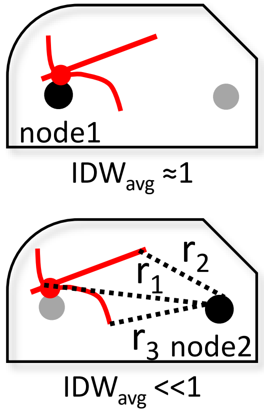
$$IDW_{avg} = \frac{1}{n}\sum_{i=1}^{p} IDW_i$$

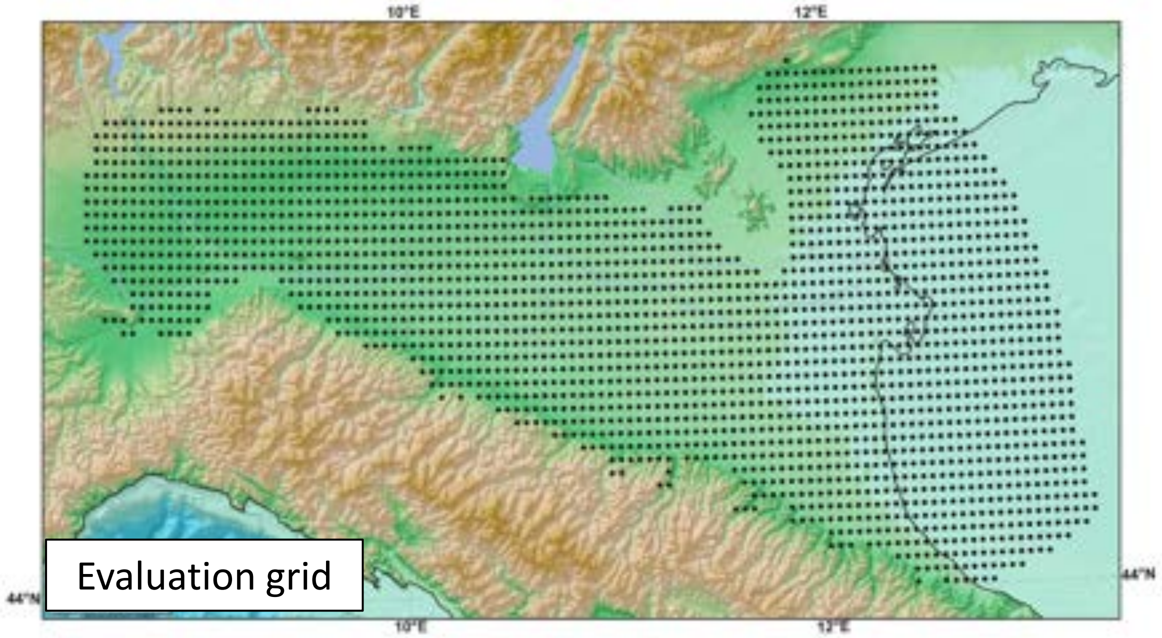
Pre-processing

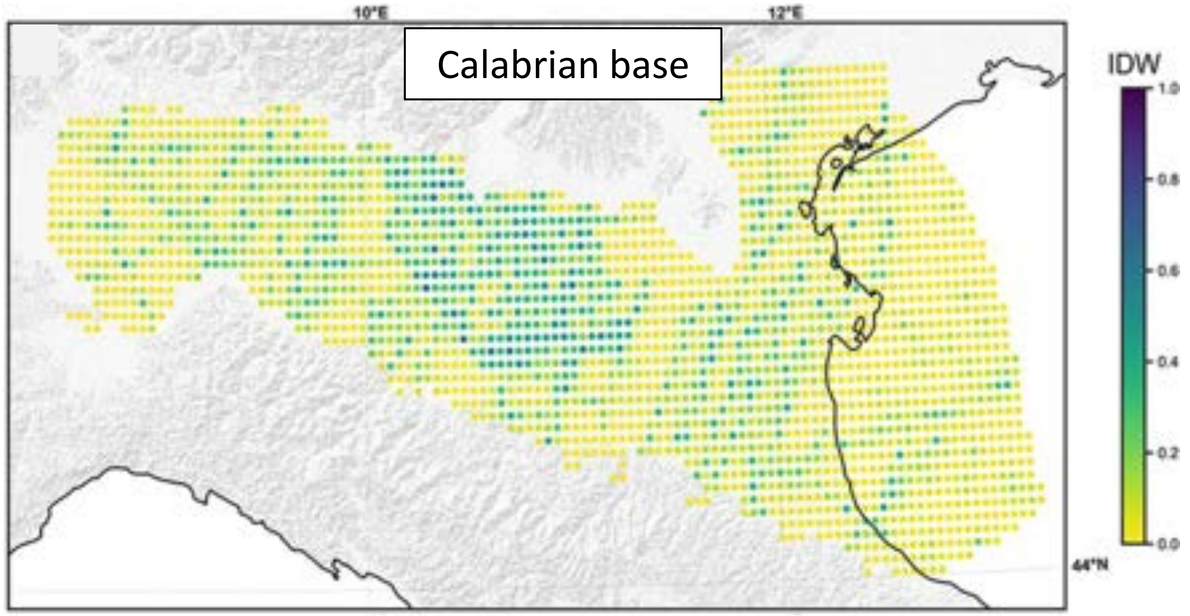
model

processing

$$\frac{1}{r^p}$$







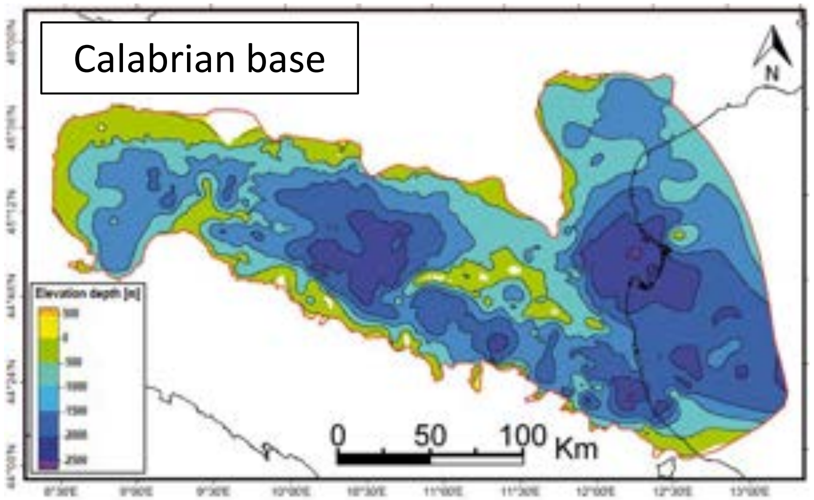
Example – vertical range of variation

Pre-processing

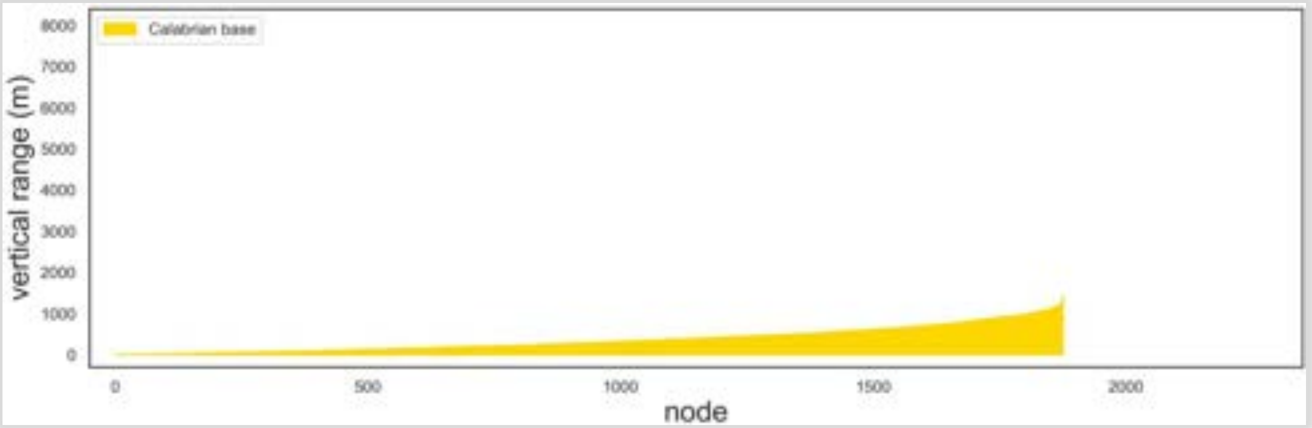
model

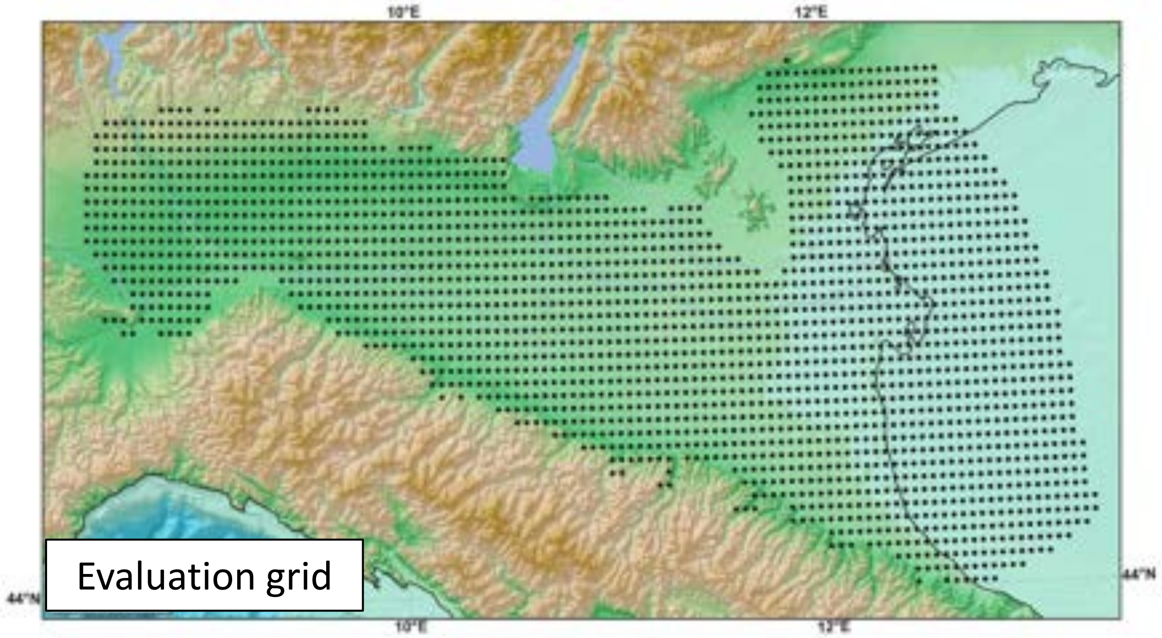
processing

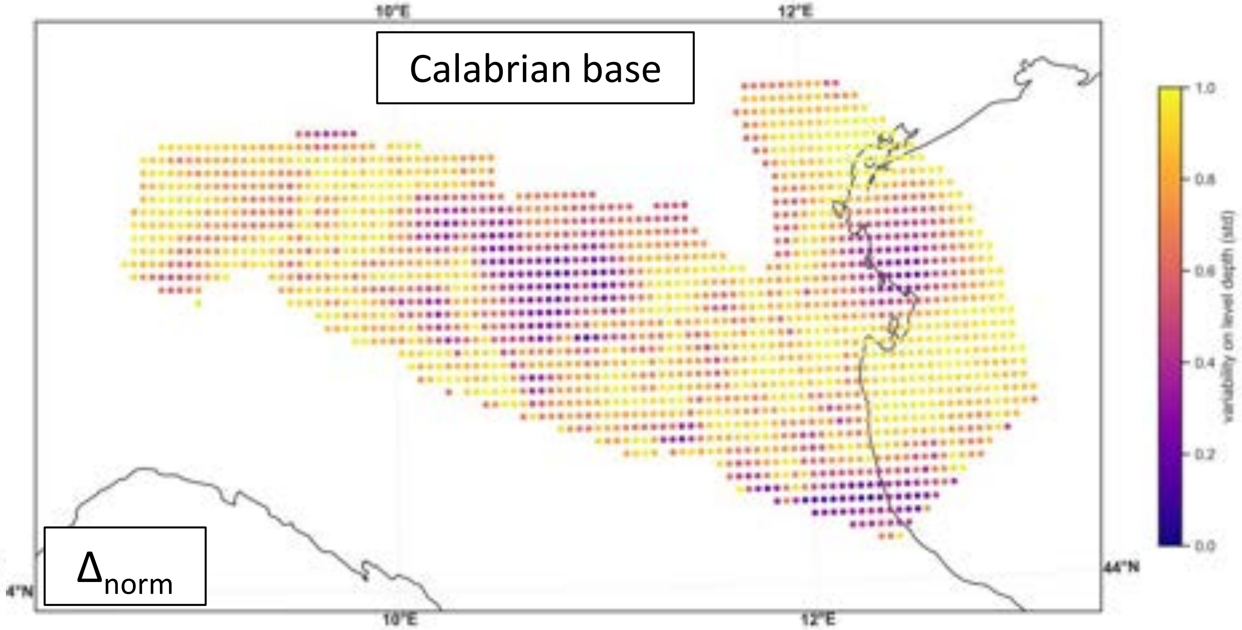
$$\frac{1}{r^p}$$

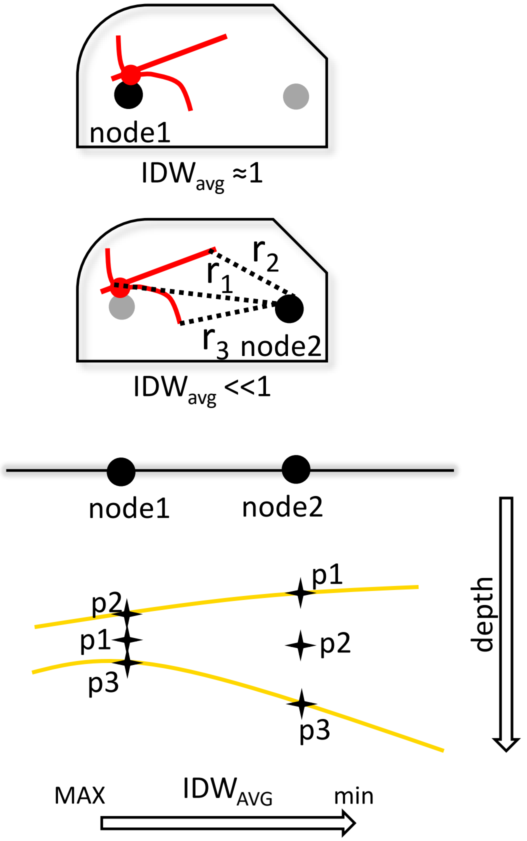


Livani et al., 2023

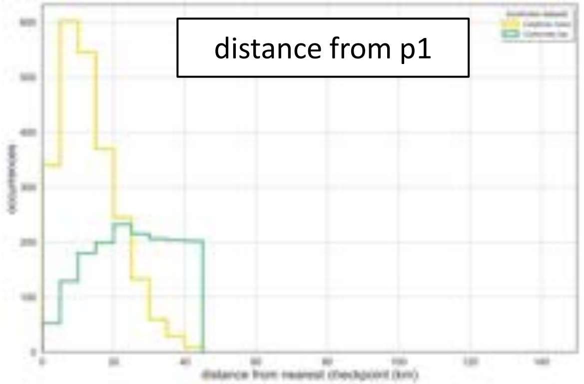




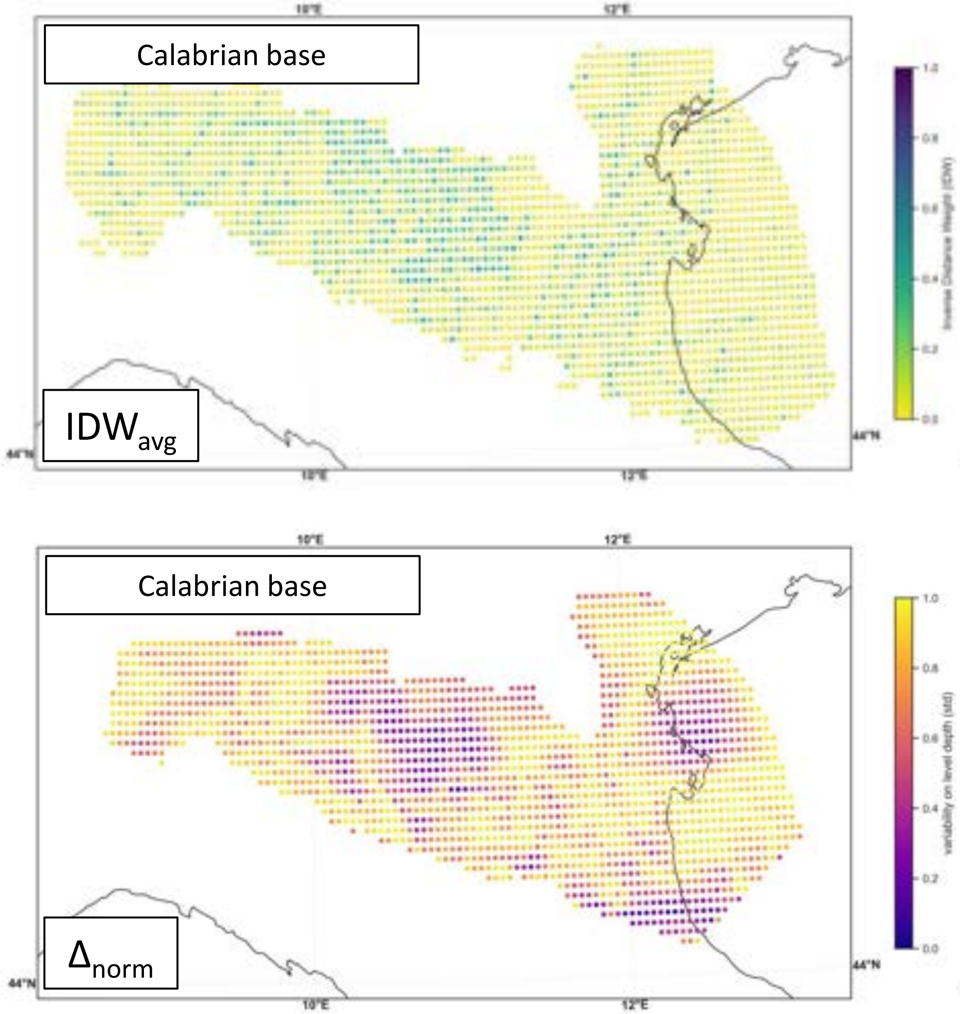




Example – comparing surfaces


distance from p1

p1 checkpoints =139

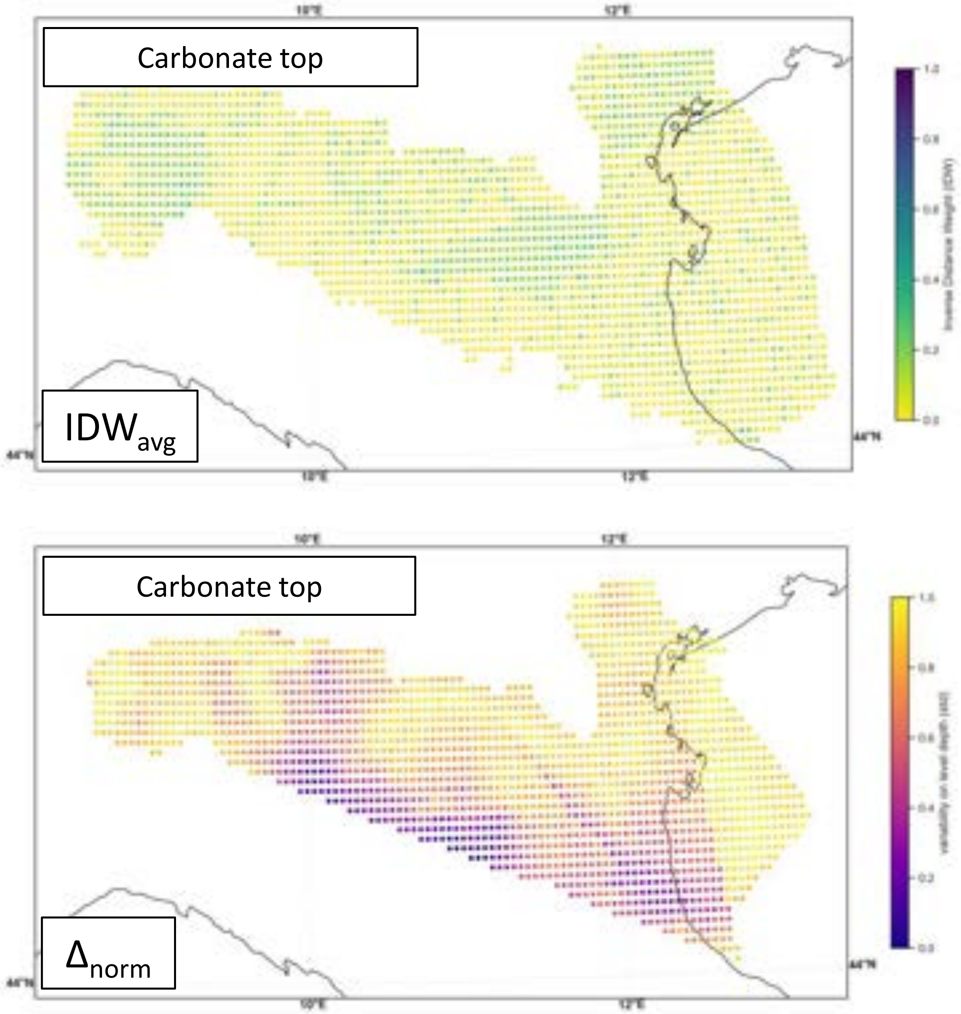

Calabrian base

IDW_{avg}

Calabrian base

Δ_{norm}

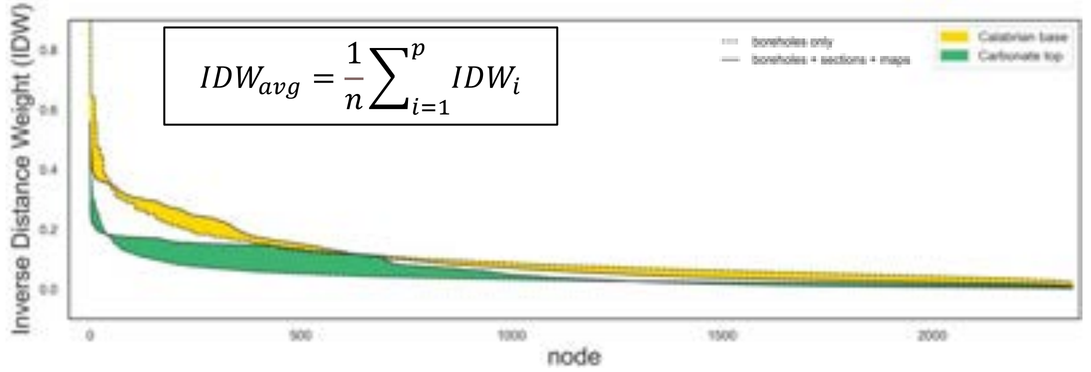
p1 checkpoints =17


Carbonate top

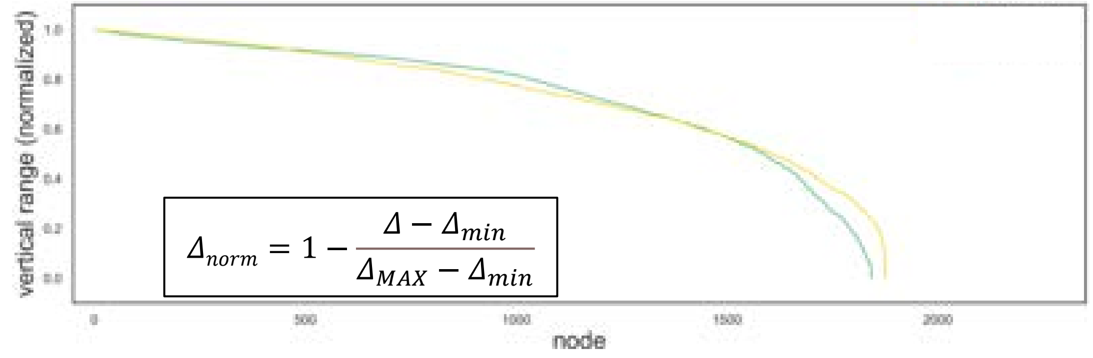
IDW_{avg}

Carbonate top

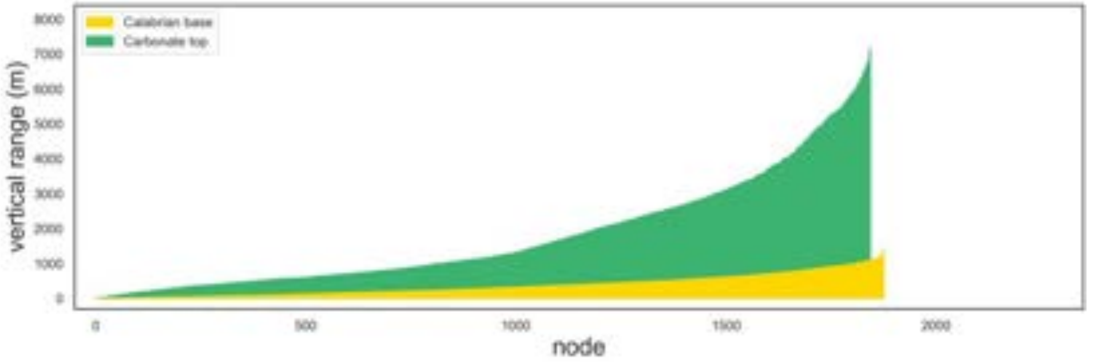
Δ_{norm}



$$IDW_{avg} = \frac{1}{n}\sum_{i=1}^{p} IDW_i$$

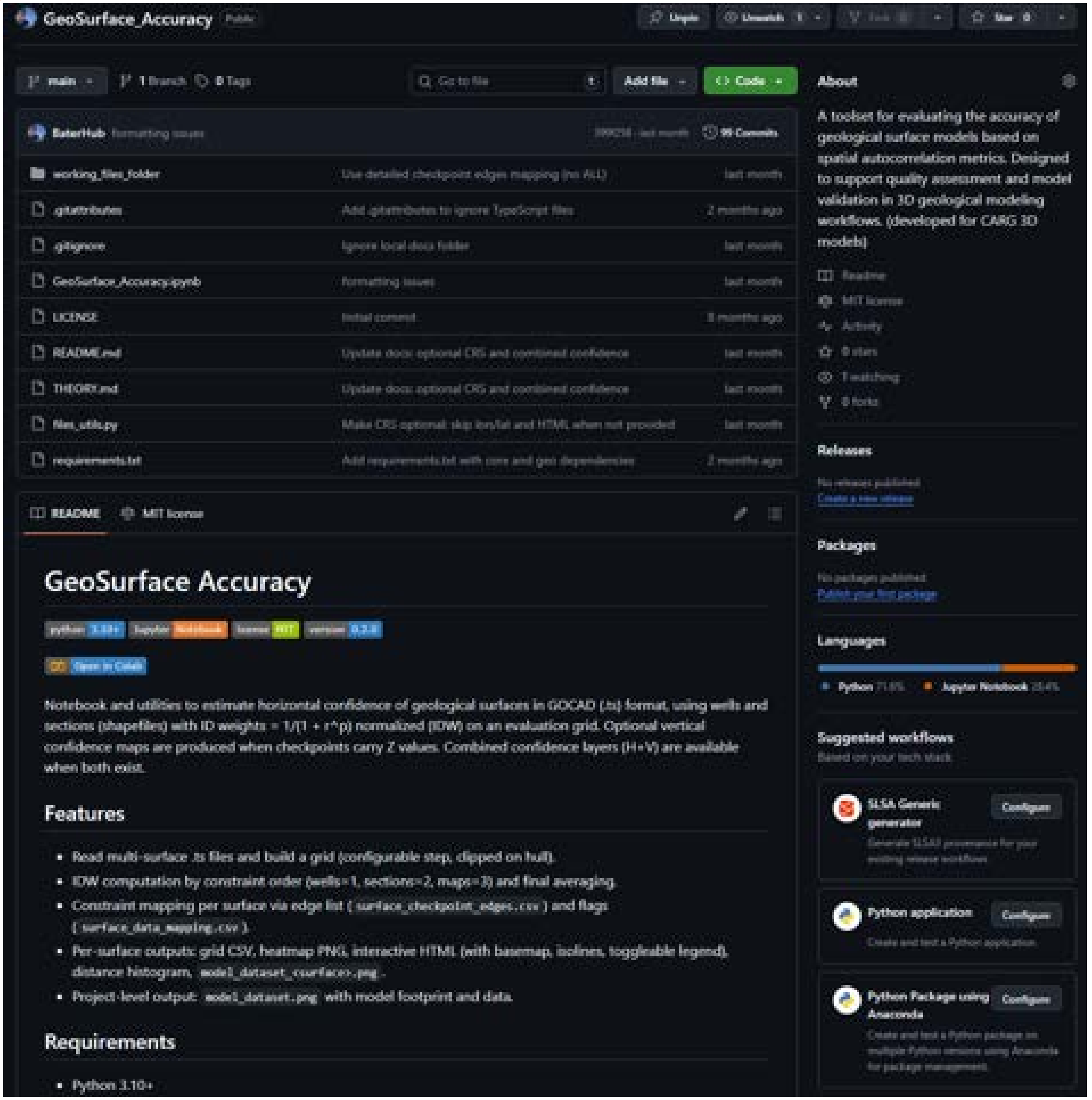


$$\Delta_{norm} = 1 - \frac{\Delta - \Delta_{min}}{\Delta_{MAX} - \Delta_{min}}$$



Livani et al., 2023

From concept to reproducible workflow



GeoSurface_Accuracy Public

main · 1 Branch · 0 Tags

BaterHub formatting issues	99 Commits	
working_files_folder	Use detailed checkpoint edges mapping (no ALL)	last month
.gitattributes	Add .gitattributes to ignore TypeScript files	2 months ago
.gitignore	Ignore local docs folder	last month
GeoSurface_Accuracy.ipynb	formatting issues	last month
LICENSE	Initial commit	8 months ago
README.md	Update docs: optional CRS and combined confidence	last month
THEORY.md	Update docs: optional CRS and combined confidence	last month
files_utils.py	Make CRS optional: skip lon/lat and HTML when not provided	last month
requirements.txt	Add requirements.txt with core and geo dependencies	2 months ago

README · MIT license

GeoSurface Accuracy

Notebook and utilities to estimate horizontal confidence of geological surfaces in GOCAD (.ts) format, using wells and sections (shapefiles) with ID weights = 1/(1 + r^p) normalized (IDW) on an evaluation grid. Optional vertical confidence maps are produced when checkpoints carry Z values. Combined confidence layers (H+V) are available when both exist.

Features

- Read multi-surface .ts files and build a grid (configurable step, clipped on hull).
- IDW computation by constraint order (wells=1, sections=2, maps=3) and final averaging.
- Constraint mapping per surface via edge list (`surface_checkpoint_edges.csv`) and flags (`surface_data_mapping.csv`).
- Per-surface outputs: grid CSV, heatmap PNG, interactive HTML (with basemap, isolines, togglable legend), distance histogram, `model_dataset_<surface>.png` .
- Project-level output: `model_dataset.png` with model footprint and data.

Requirements

- Python 3.10+

About

A toolset for evaluating the accuracy of geological surface models based on spatial autocorrelation metrics. Designed to support quality assessment and model validation in 3D geological modeling workflows. (developed for CARG 3D models)

Releases

No releases published

Packages

No packages published

Languages

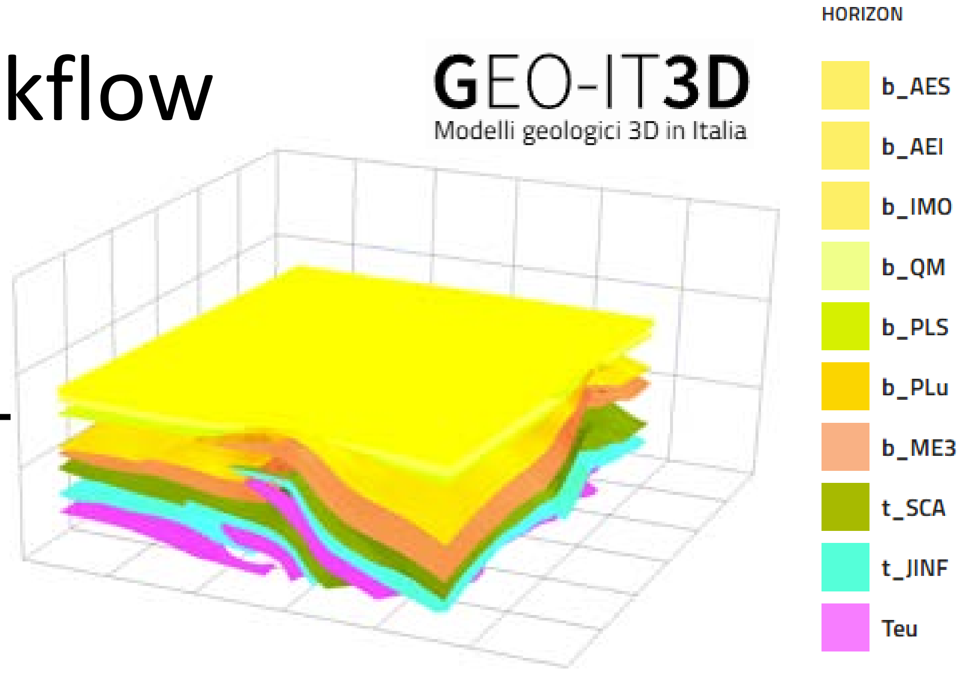
Python · Jupyter Notebook

Suggested workflows

SLSA Generic generator · Python application · Python Package using Anaconda

https://github.com/BaterHub/GeoSurface_Accuracy

GEO-IT3D
Modelli geologici 3D in Italia



https://geo-it3d.isprambiente.it/

§INPUT FILES format:
- GOCAD .ts (structured surfaces)
- ESRI Shapefile .shp
- Tabular data .csv, .txt

§OUTPUT FILES:
- confidence maps .png
- numerical outcomes .csv
- statistics .csv

-> Open and reproducible Python notebook
-> Based on interoperable formats
-> Horizontal component fully implemented
-> Vertical component under development

Conclusions

i) **Transparent and reproducible confidence mapping**
ii) **Spatially explicit, data-driven approach**
iii) **Designed for heterogeneous Geological Survey datasets**

Open points

i) **Sensitivity analysis (grid resolution/search radius)**
ii) **Systematic analysis of several case studies**
iii) **Comparison with alternative spatial models**
iv) **Integration of horizontal and vertical confidence**

Thanks for listening

https://github.com/BaterHub/GeoSurface_Accuracy

* patrizio.petricca@isprambiente.it

Advancing probabilistic uncertainty-incorporated 3D voxel modelling – the application of uncertainty

Thomas Højland Lorentzen

Anne-Sophie Høyer

Rasmus Bødker Madsen (Presenter)

GSEU workshop: Exploring, Quantifying and Communicating Uncertainties in Geological Models

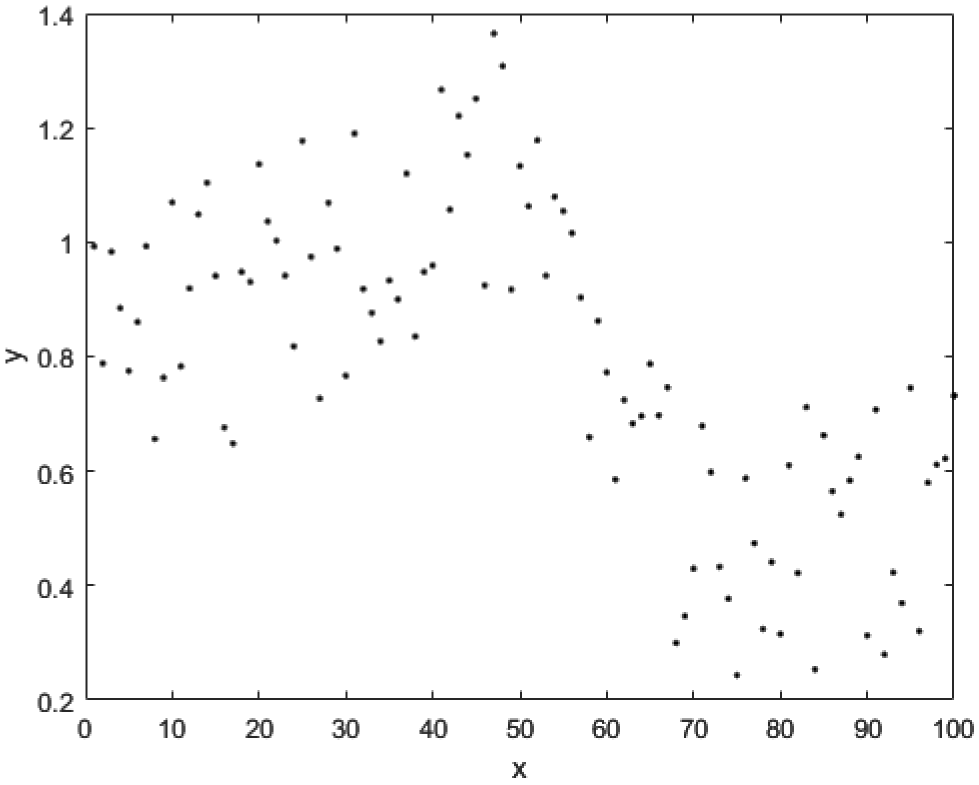
GEUS

Data Don't Tell the Whole Story

Local measurements only

No context between observations

No structure



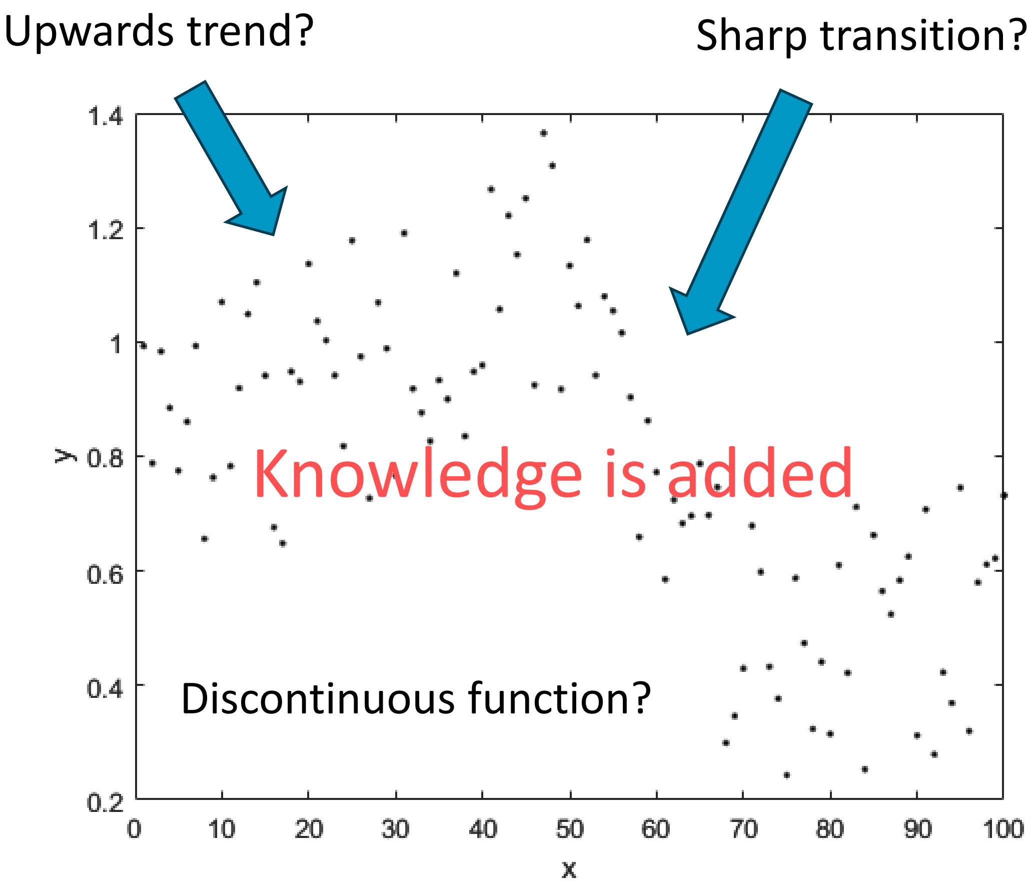
Models Give Context to Data

Connects data

Interpret structure

Generalize beyond measurements

Model = data + interpretation + assumption



Models Give Context to Data

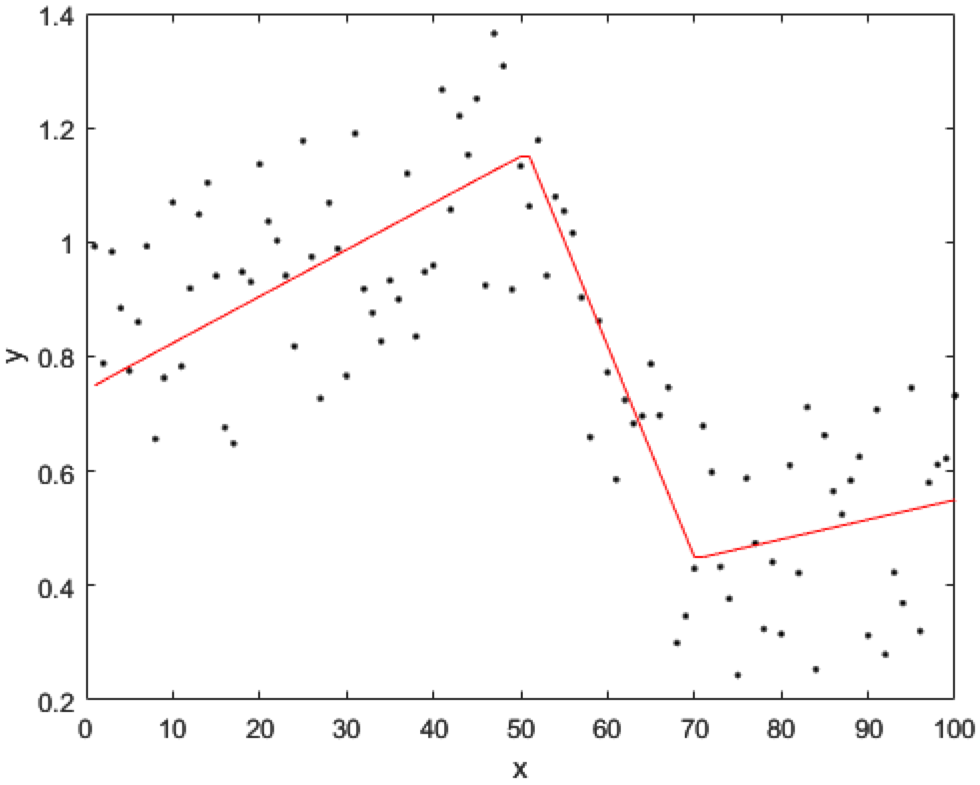
Connects data

Interpret structure

Generalize beyond measurements

Model = data + interpretation + assumption

“Model representation” to convey information

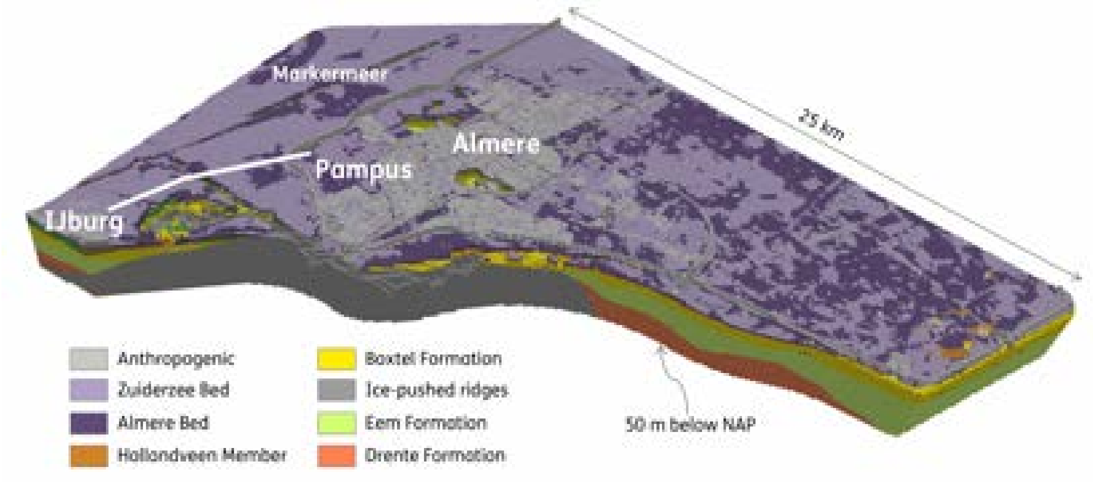


G E U S

Model representations are key for communication! – Especially in geoscience

Example: GEOTOP

- Netherlands
- National-scale voxel model
- Multiple applications
- Working tool
- Communication with stakeholders and end-users
    - Knowledge ingrained (“self explanatory”)

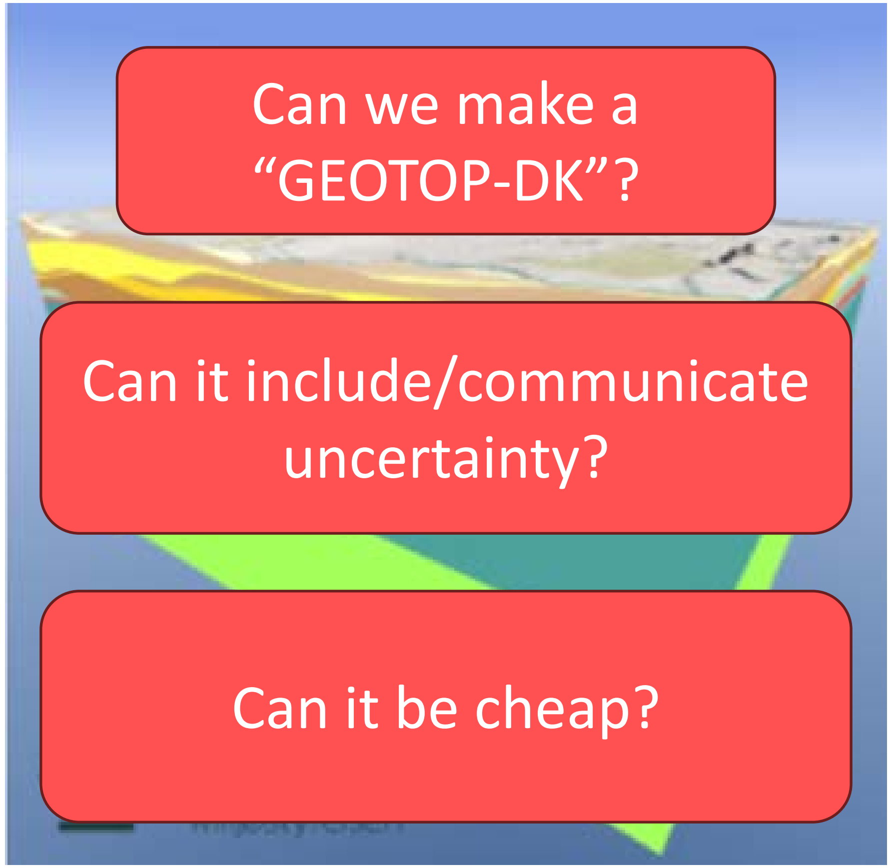


https://www.dinoloket.nl/en/nieuws/geotop-extended-to-almere

Motivation: National voxel model of Denmark

Today: Hydrostratigraphic model
- Variable quality
  - Lack of near surface resolution
  - Variable modeling strategies
  - Variable data availability
- Not fit for multipurpose use

- Unused subsurface data



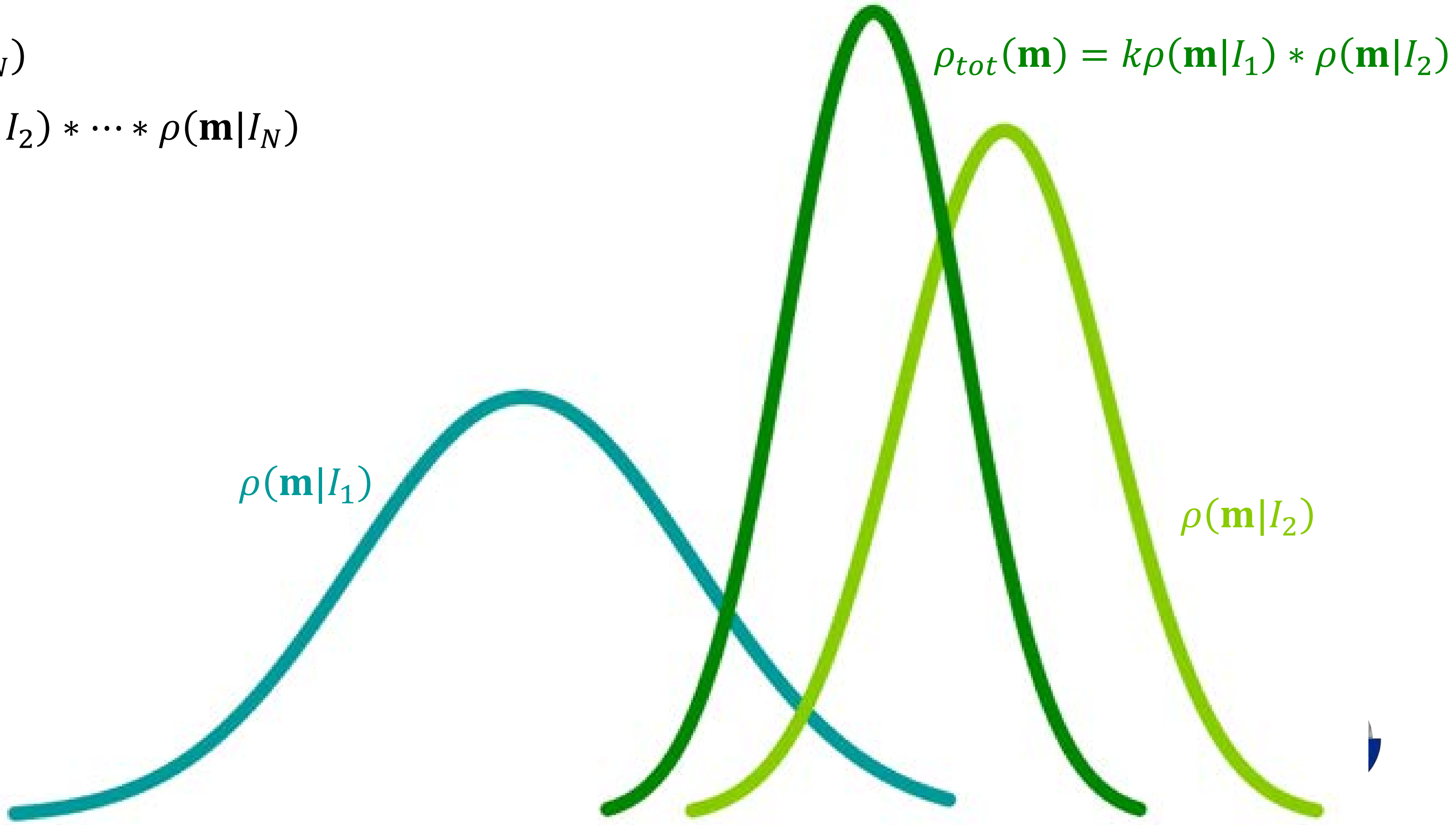
Can we make a “GEOTOP-DK”?

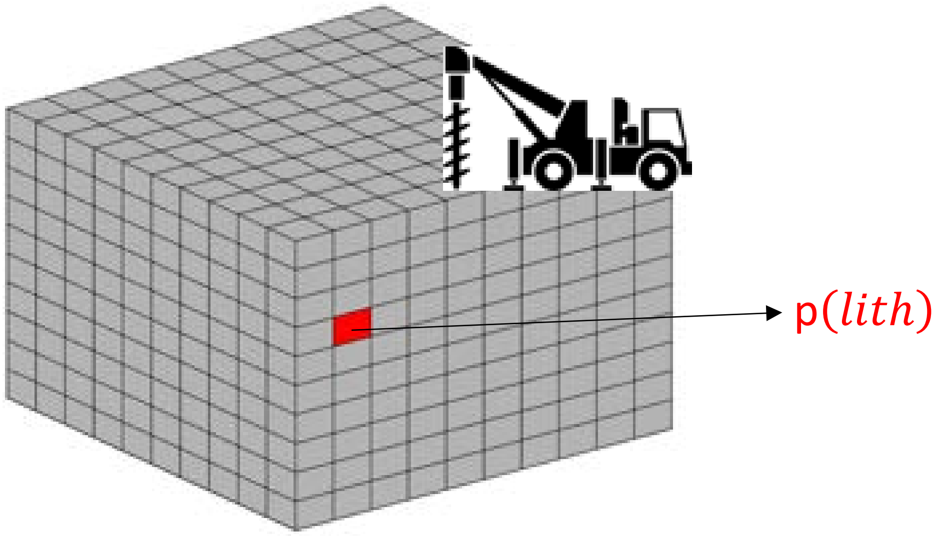
Can it include/communicate uncertainty?

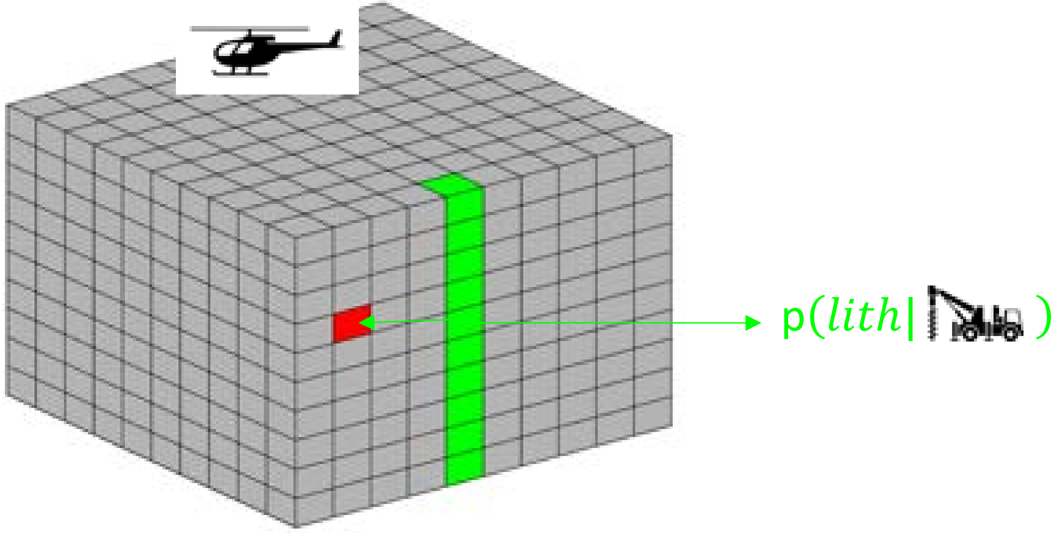
Can it be cheap?

The answer: Probabilistic data integration

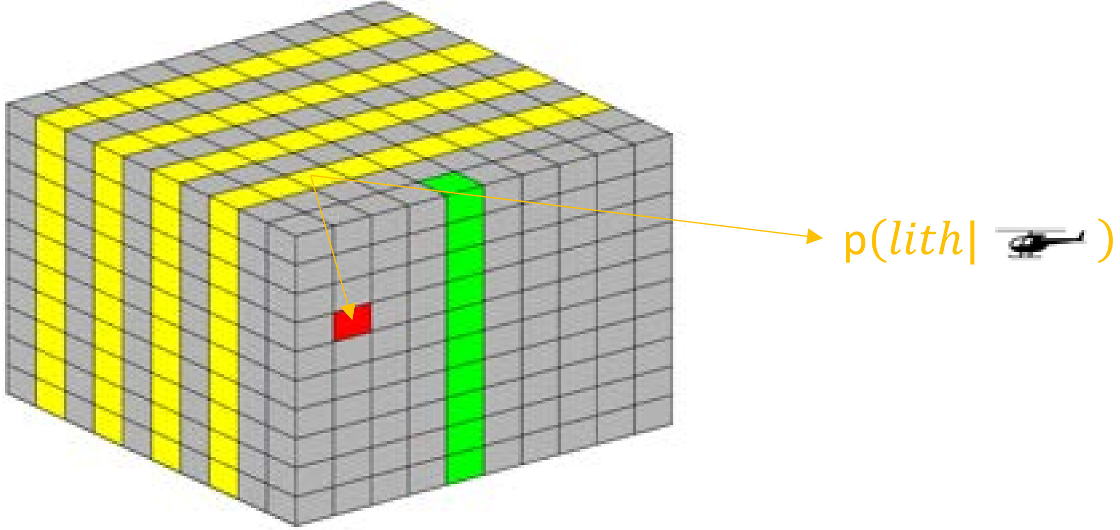
$$\begin{aligned}\rho_{tot}(\mathbf{m}) &= k\rho(\mathbf{m}|I_1, I_2, \dots, I_N) \\ &= k\rho(\mathbf{m}|I_1) * \rho(\mathbf{m}|I_2) * \cdots * \rho(\mathbf{m}|I_N)\end{aligned}$$







$$p(lith|\text{🏗️} \,\&\, \text{🚁}) = k\, p(lith|\text{🏗️}) * p(lith|\text{🚁}) * p(lith|I_3) \ldots p(lith|I_n)$$



Challenge!

1. How to **describe/translate** all subsurface Information (with uncertainty) as probability
2. How to make geologically informed **extrapolation** of the information

Two new concepts

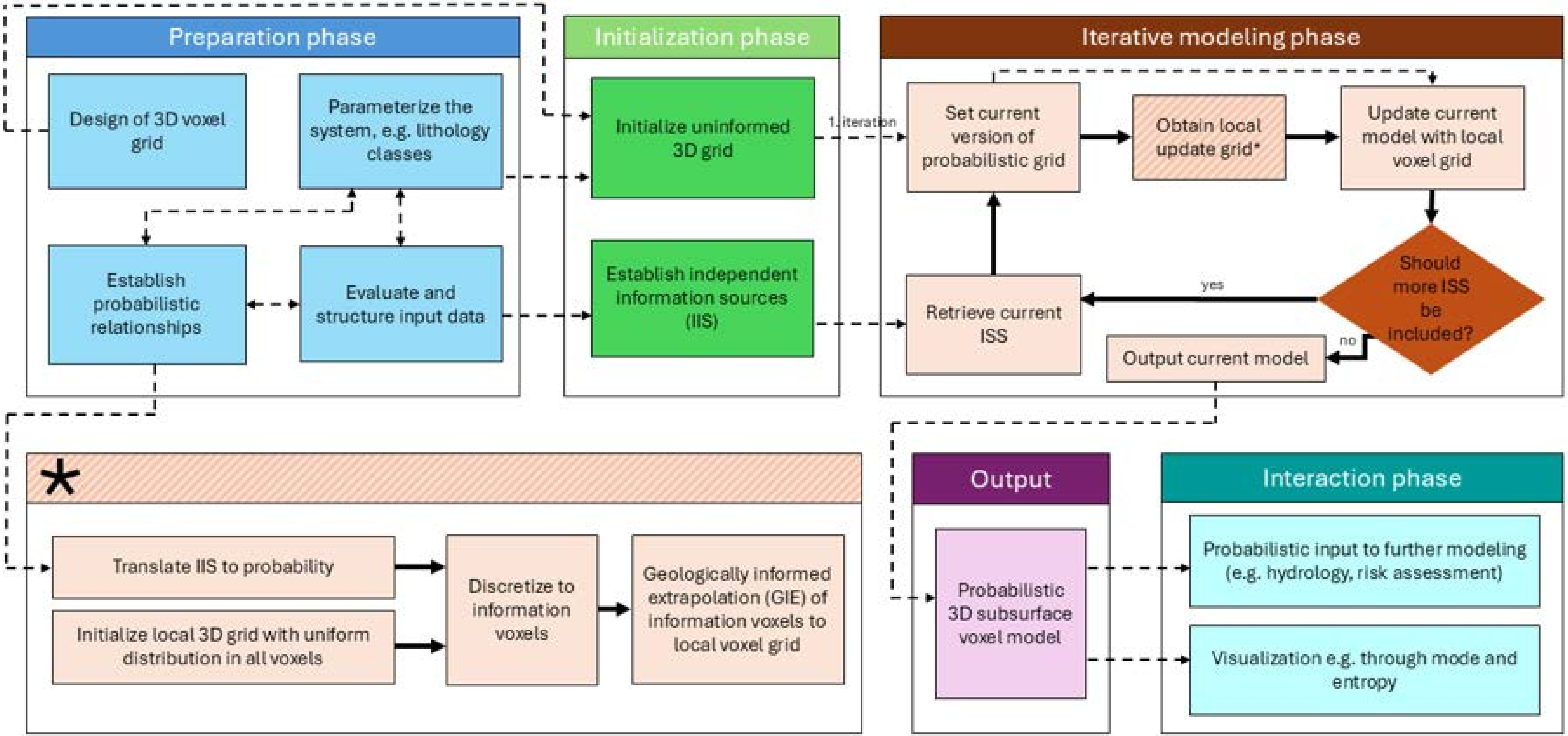
Independent Information Sources (IIS)

- Self-contained units of subsurface information (e.g. boreholes, geophysics, interpretations)
- Translated into voxel-scale probability distributions with explicit uncertainty
- Assumed conditionally independent, enabling systematic combination and local updates

Geologically Informed Extrapolation (GIE)

- Mechanism for spatially propagating IIS information into the 3D voxel grid
- Based on geological reasoning rather than statistical interpolation
- Defines controlled spatial influence in a transparent and efficient way

Workflow



Preparation phase

Design of 3D voxel grid

Parameterize the system, e.g. lithology classes

Establish probabilistic relationships

Evaluate and structure input data

Initialization phase

Initialize uninformed 3D grid

Establish independent information sources (IIS)

Iterative modeling phase

Set current version of probabilistic grid

Obtain local update grid*

Update current model with local voxel grid

Should more ISS be included?

Retrieve current ISS

Output current model

*****

Translate IIS to probability

Initialize local 3D grid with uniform distribution in all voxels

Discretize to information voxels

Geologically informed extrapolation (GIE) of information voxels to local voxel grid

Output

Probabilistic 3D subsurface voxel model

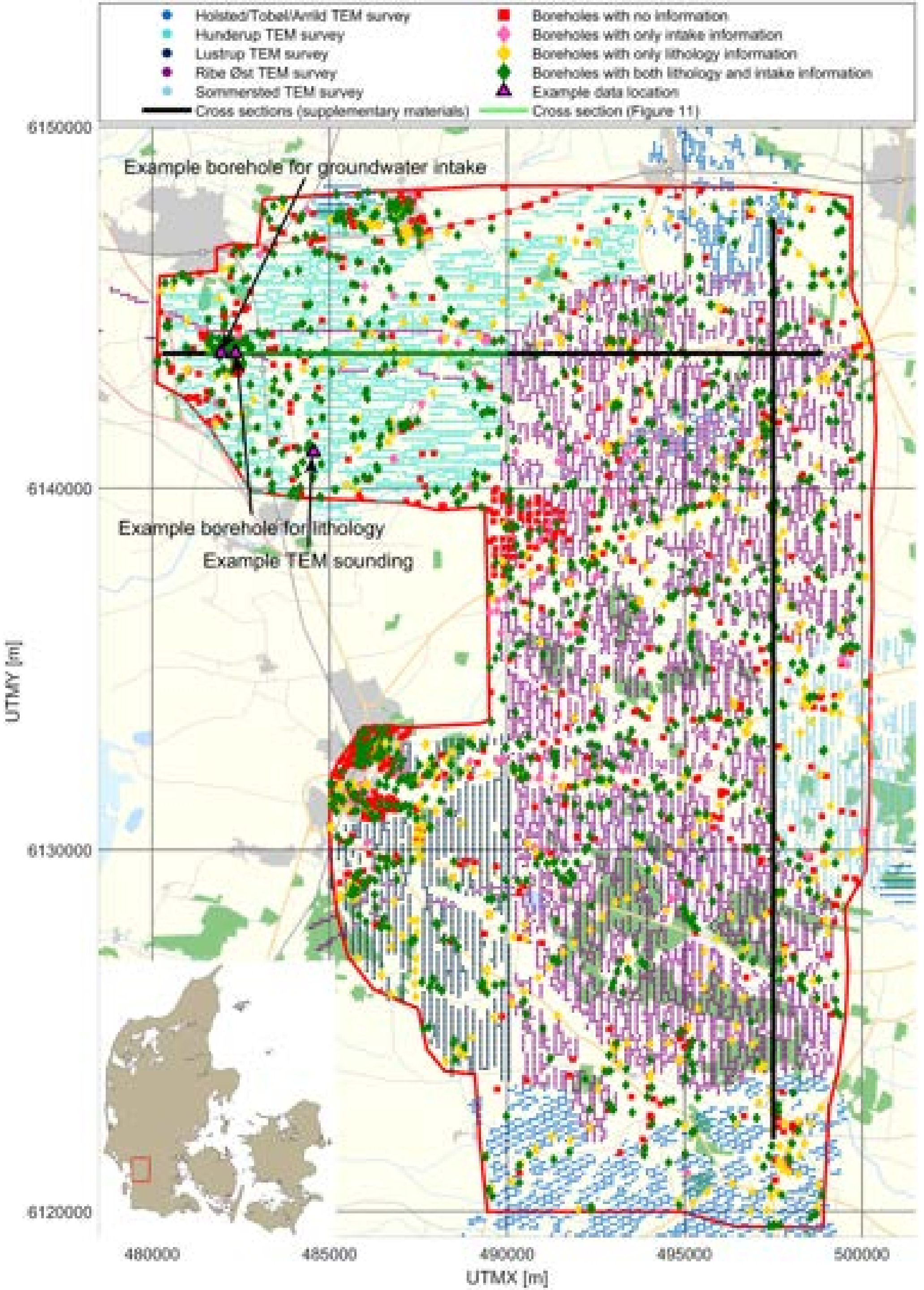
Interaction phase

Probabilistic input to further modeling (e.g. hydrology, risk assessment)

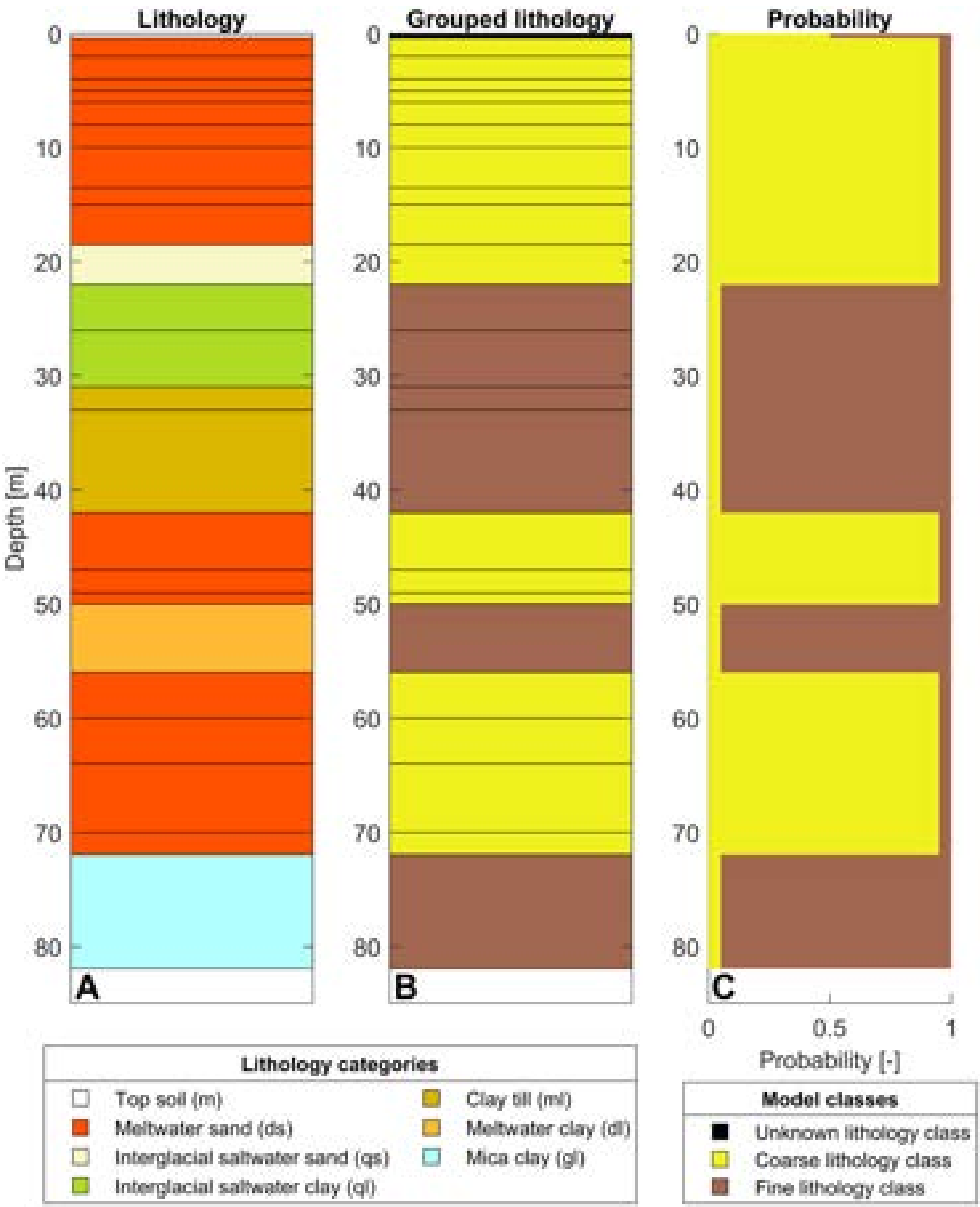
Visualization e.g. through mode and entropy

Example: Hydrogeological modeling Ribe, Denmark

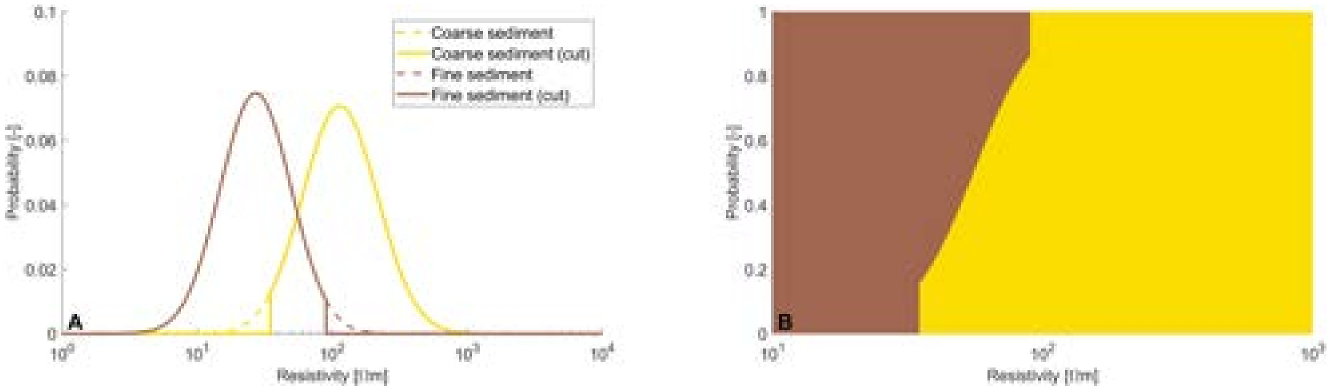
- The heterogenous Saalian unit was modeled using the proposed voxel modeling framework
- Data sources
  - Boreholes
  - SkyTEM surveys
  - Water extraction

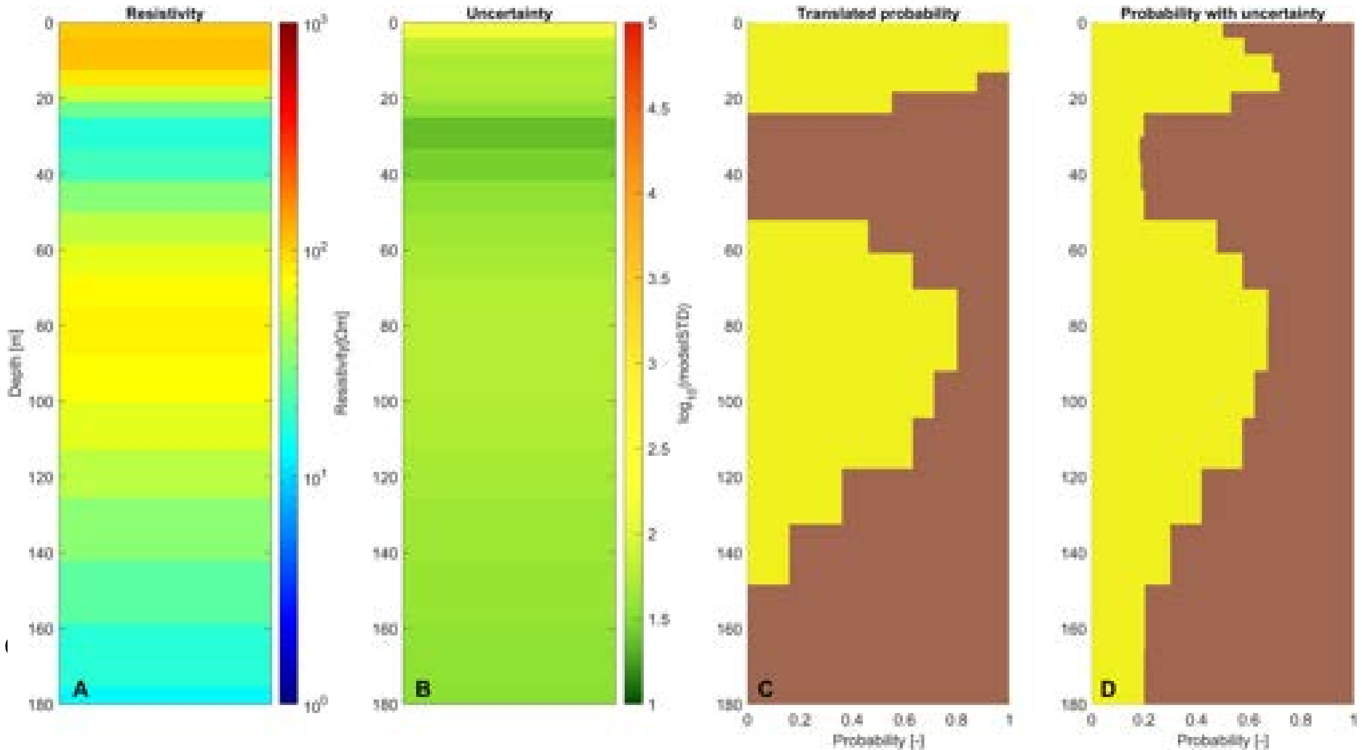


Independent Information Sources (IIS)

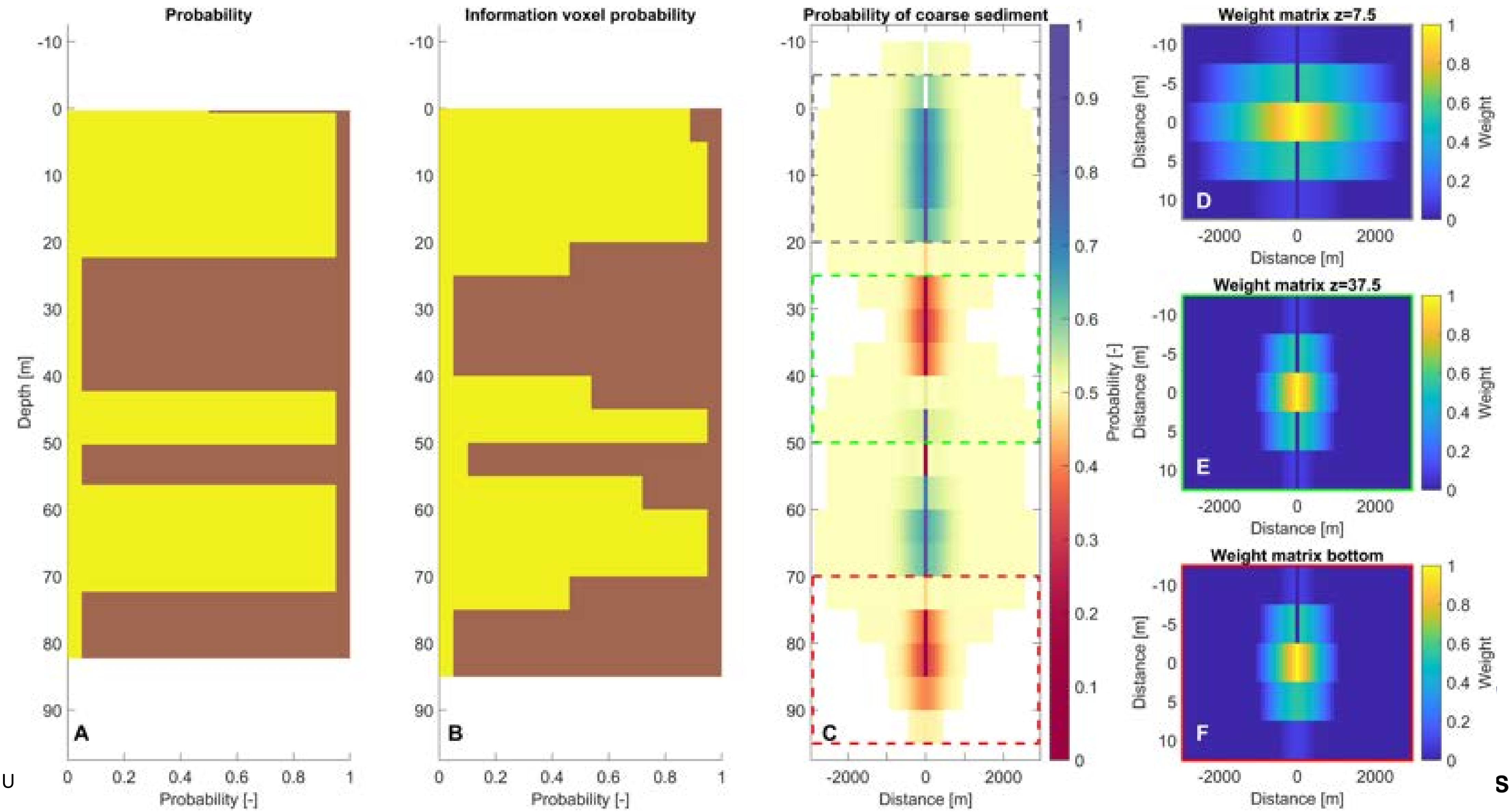


tainties in (

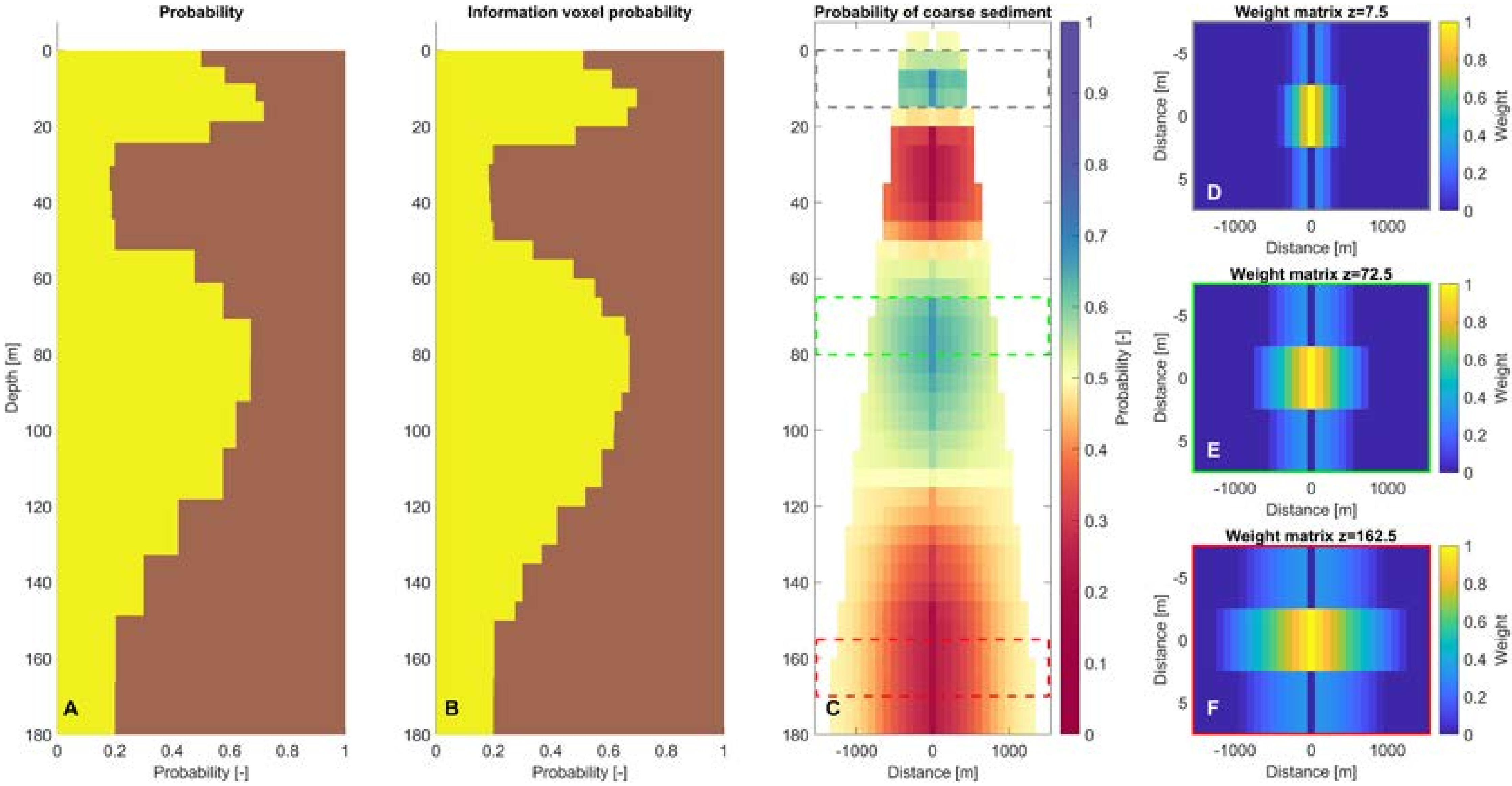


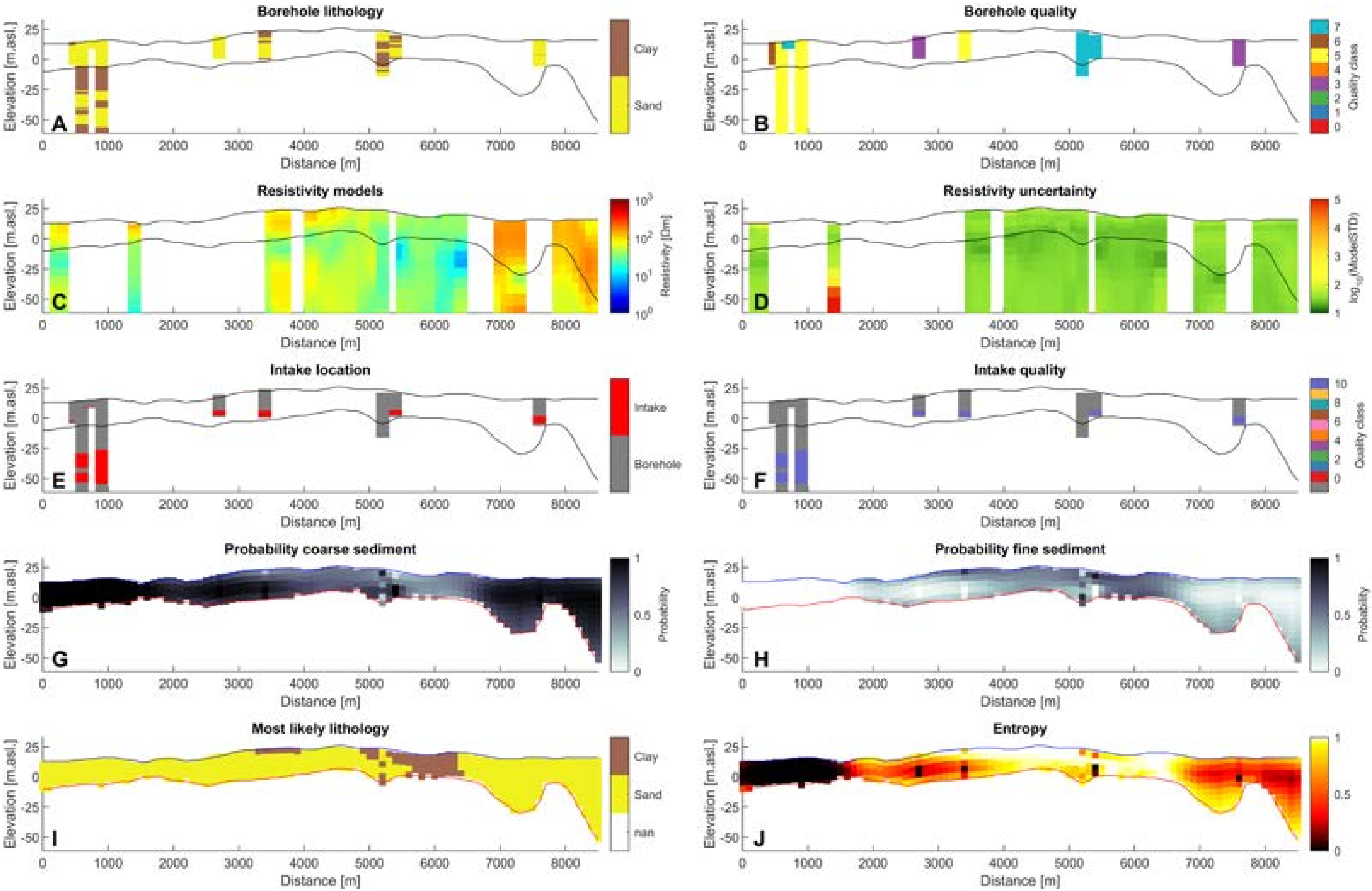


Geologically Informed Extrapolation (GIE) - Borehole



Geologically Informed Extrapolation (GIE) - SkyTEM




Borehole lithology
Borehole quality
Resistivity models
Resistivity uncertainty
Intake location
Intake quality
Probability coarse sediment
Probability fine sediment
Most likely lithology
Entropy
A
B
C
D
E
F
G
H
I
J
Elevation [m.asl.]
Distance [m]
25
0
-25
-50
0
1000
2000
3000
4000
5000
6000
7000
8000
Clay
Sand
nan
Quality class
7
6
5
4
3
2
1
0
10
8
Resistivity [Ωm]
10^3
10^2
10^1
10^0
$\log_{10}$(ModelSTD)
Intake
Borehole
Probability
0.5
1

Describe information as probability distributions of the model parameters

- We have considered:
    - Boreholes
        - Lithology
        - Water production
    - TEM (SkyTEM, tTEM)
    - Surface geology maps

- Any subsurface information can in theory be used if a relation to chosen model parameters can be established

Geologically informed extrapolation of the information

- We have considered:
    - Simple geological knowledge
        - Shape and weight are completely free to design
    - Geophysical method based extrapolation
        - TEM sensitivity functions

- The modeling framework is adaptable to any spatial information available

Paper submitted to Engineering Geology

Title: Advancing probabilistic uncertainty-incorporated 3D voxel modelling – the application of uncertainty

Thank you

How are uncertainties taken into account in the SPDE process?

Charlie GARAYT(1,2), Nicolas Desassis (1), Nicolas Clausolles(2),
Simon Lopez(2)

(1) Mines Paris, PSL
(2) BRGM

02/03/2026

What is SPDE? (Lindgren and Rue, 2011)

SPDE: stochastic partial differential equation

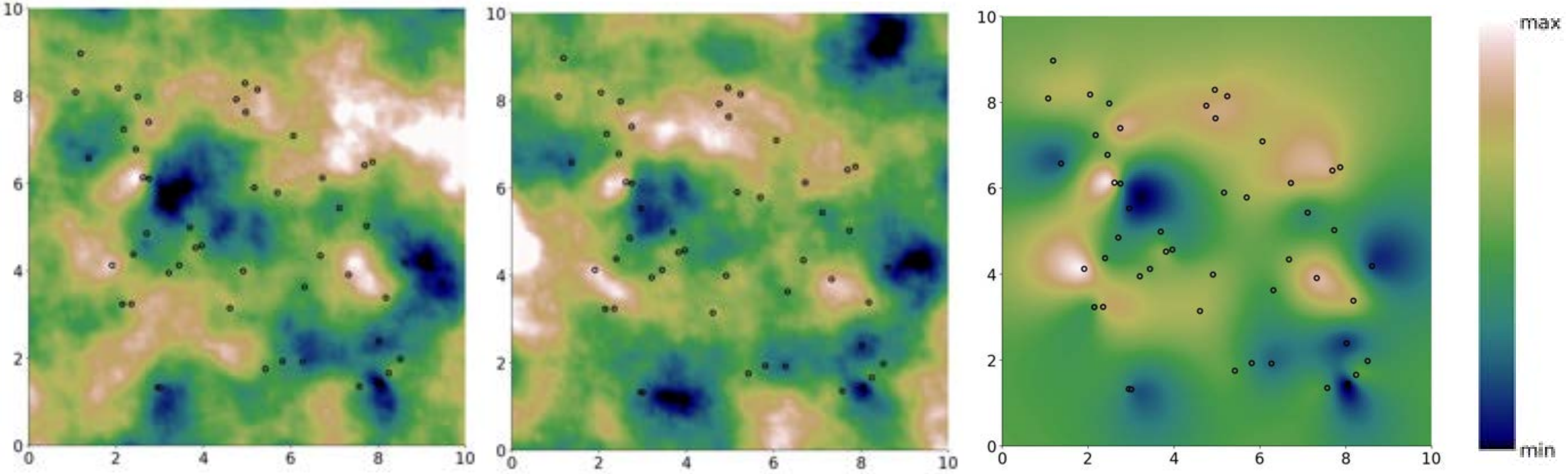
$$(\kappa^2\text{-}\Delta)^{\alpha/2}\ \mathrm{Z} = \overbrace{\mathrm{W}}^{\text{Gaussian white noise}}$$

What is SPDE? (Lindgren and Rue, 2011)

SPDE: stochastic partial differential equation

$$(\kappa^2\text{-}\Delta)^{\alpha/2}\overbrace{\mathrm{Z}}^{\text{What we are looking for}} = \overbrace{\mathrm{W}}^{\text{Gaussian white noise}}$$

Z: a Gaussian random field (GRF)



Simulation 1 Simulation 2 Kriging (simulations mean)

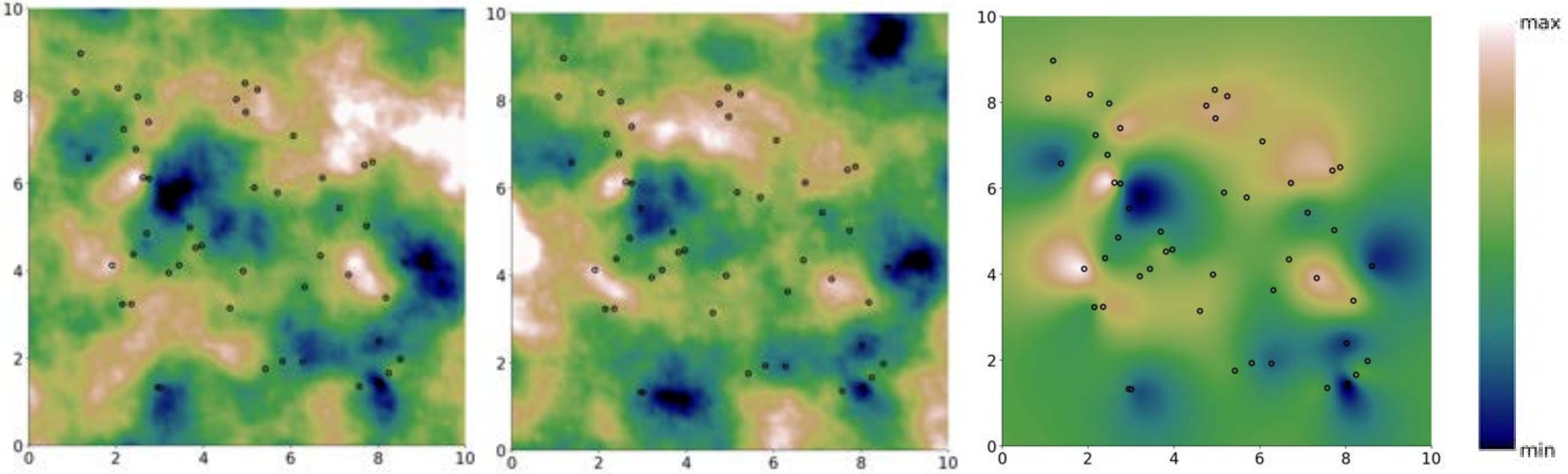
What is SPDE? (Lindgren and Rue, 2011)

SPDE: stochastic partial differential equation

$$(\underbrace{\kappa}_{}^{2}\text{-}\Delta)^{\underbrace{\alpha}_{}/2}\overbrace{\mathrm{Z}}^{\text{What we are looking for}}=\overbrace{\mathrm{W}}^{\text{Gaussian white noise}}$$

Two parameters > 0

Z: a Gaussian random field (GRF)



Simulation 1 Simulation 2 Kriging (simulations mean)

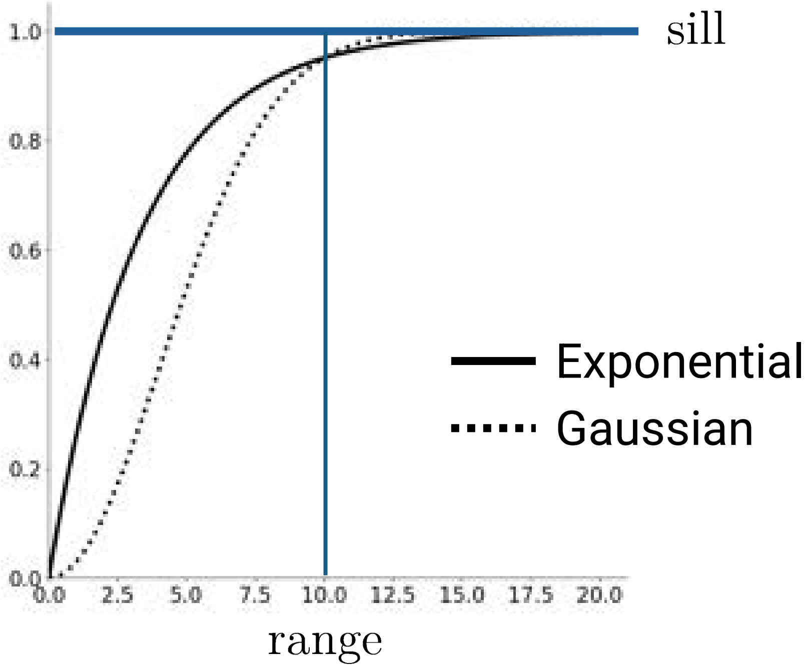
Computation of a Gaussian random field

“Classic” geostatistics, covariance approach

1. Definition of a covariance/variogram model from data
2. Computation of the covariance matrix
3. Inversion of the covariance matrix

Computation time function of n_{data} ($O(n^3)$)

Variogram model



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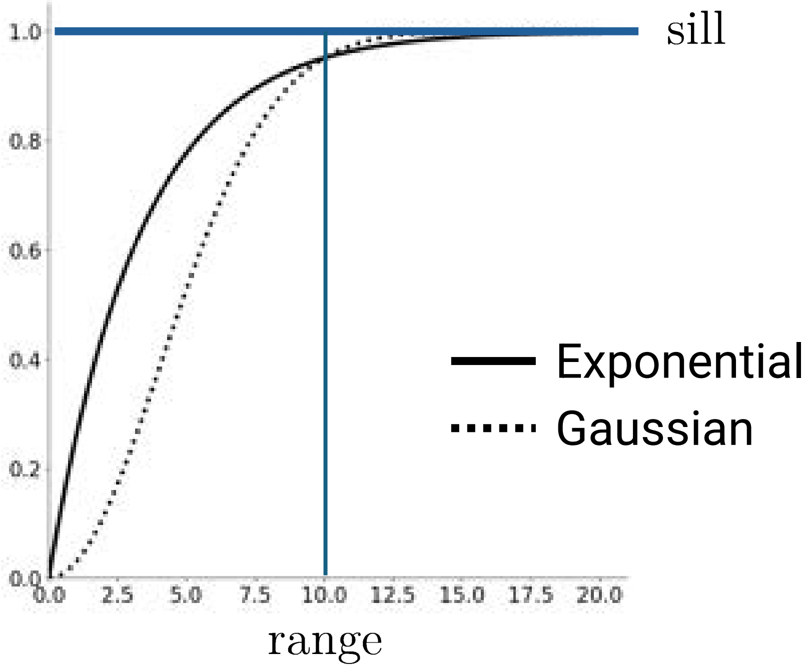
Computation time function of n_{data} ($O(n^3)$)

SDPE approach

1. Definition of parameters κ and α (see next slide)
2. Definition of an underlying mesh for finite element method (FEM)
3. Computation of the precision matrix (inverse of the covariance matrix) by solving the SPDE with FEM

Computation time not function of n_{data}



Variogram model

Link between κ and α and variogram models

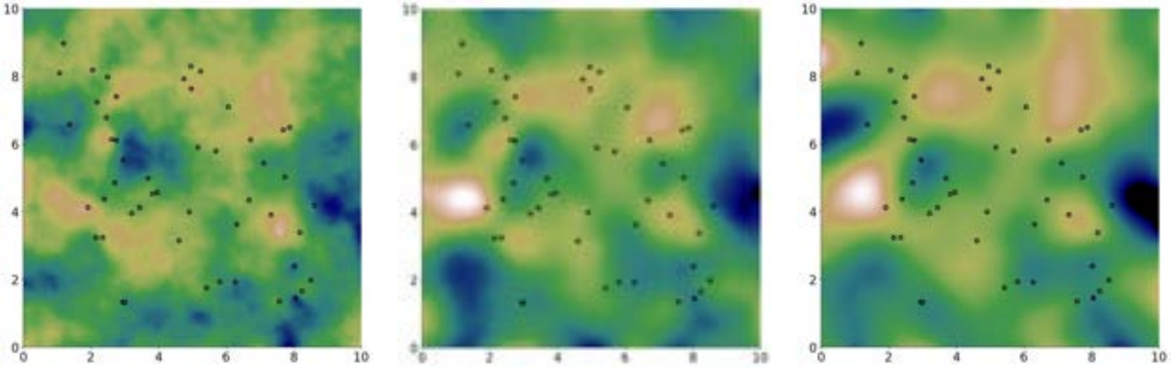
Solution Z of the SDPE $(\kappa^2\text{-}\Delta)^{\alpha/2}\ \mathrm{Z} = \mathrm{W}$ is a GRF parametrized by a Matérn covariance

(Whittle, 1954)

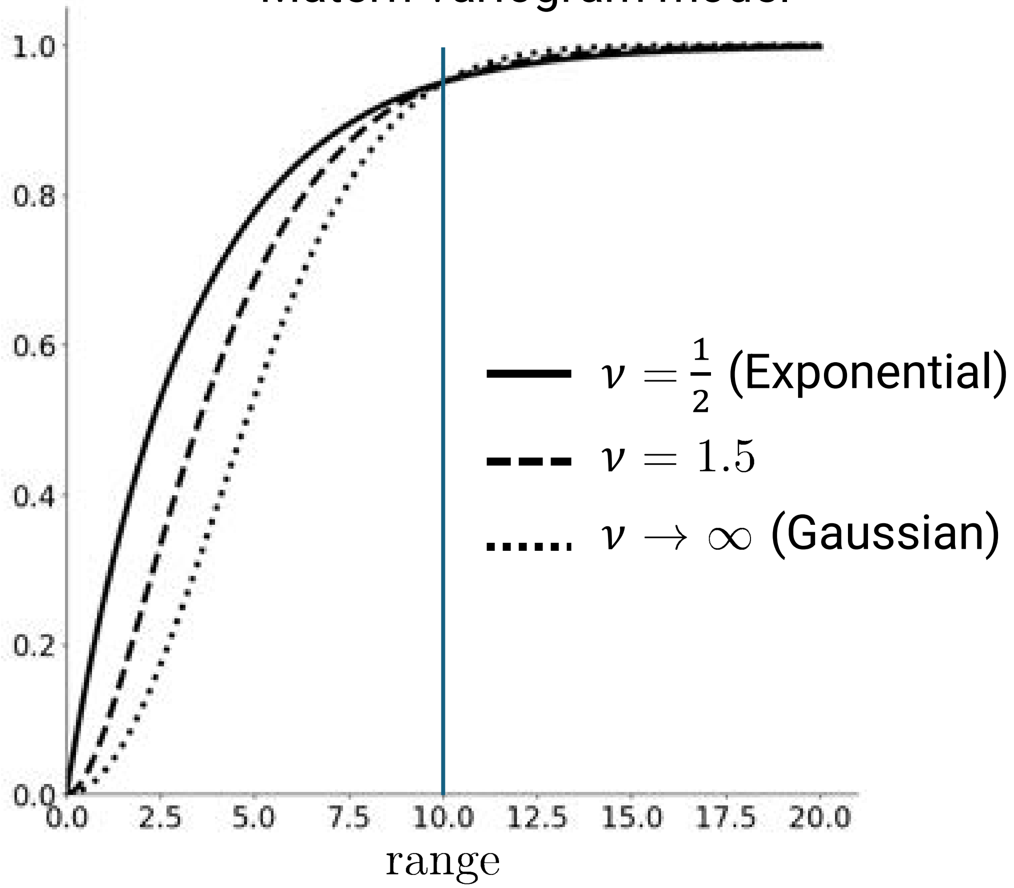
Link between κ and α and variogram models

Solution Z of the SDPE $(\kappa^2\text{-}\Delta)^{\alpha/2}\ \mathrm{Z} = \mathrm{W}$ is a GRF parametrized by a Matérn covariance

➔Equivalence between the SPDE approach and the covariance approach (Whittle, 1954)



$\nu = 1$ $\nu = 2$ $\nu = 3$



Matérn variogram model

Link between κ and α and variogram models

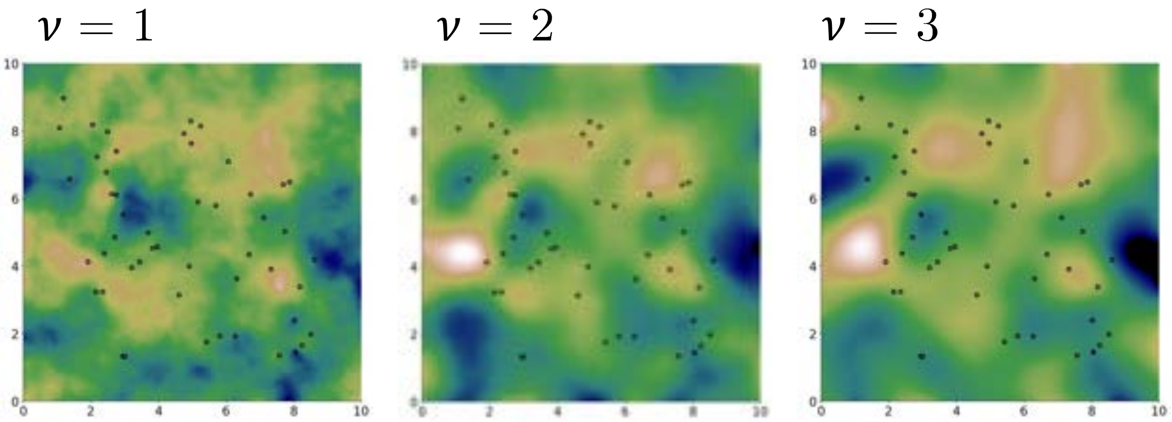
Solution Z of the SDPE $(\kappa^2\text{-}\Delta)^{\alpha/2}\ \mathrm{Z} = \mathrm{W}$ is a GRF parametrized by a Matérn covariance

(Whittle, 1954)

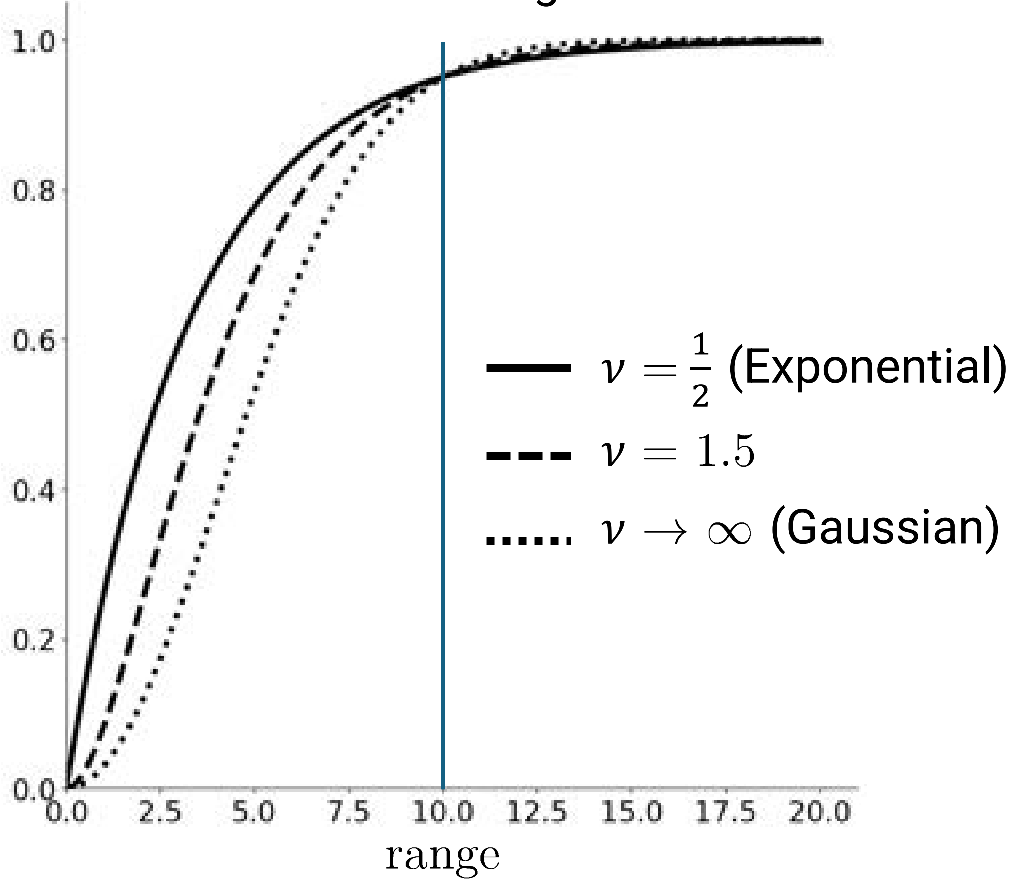
- ➔ Equivalence between the SPDE approach and the covariance approach
- ➔ SPDE parameters have a physical interpretation

$\nu = \alpha$ - $\frac{d}{2}$ smoothness | d: dimension

$\kappa \propto \frac{1}{range}$


$\nu = 1$ $\nu = 2$ $\nu = 3$

Matérn variogram model



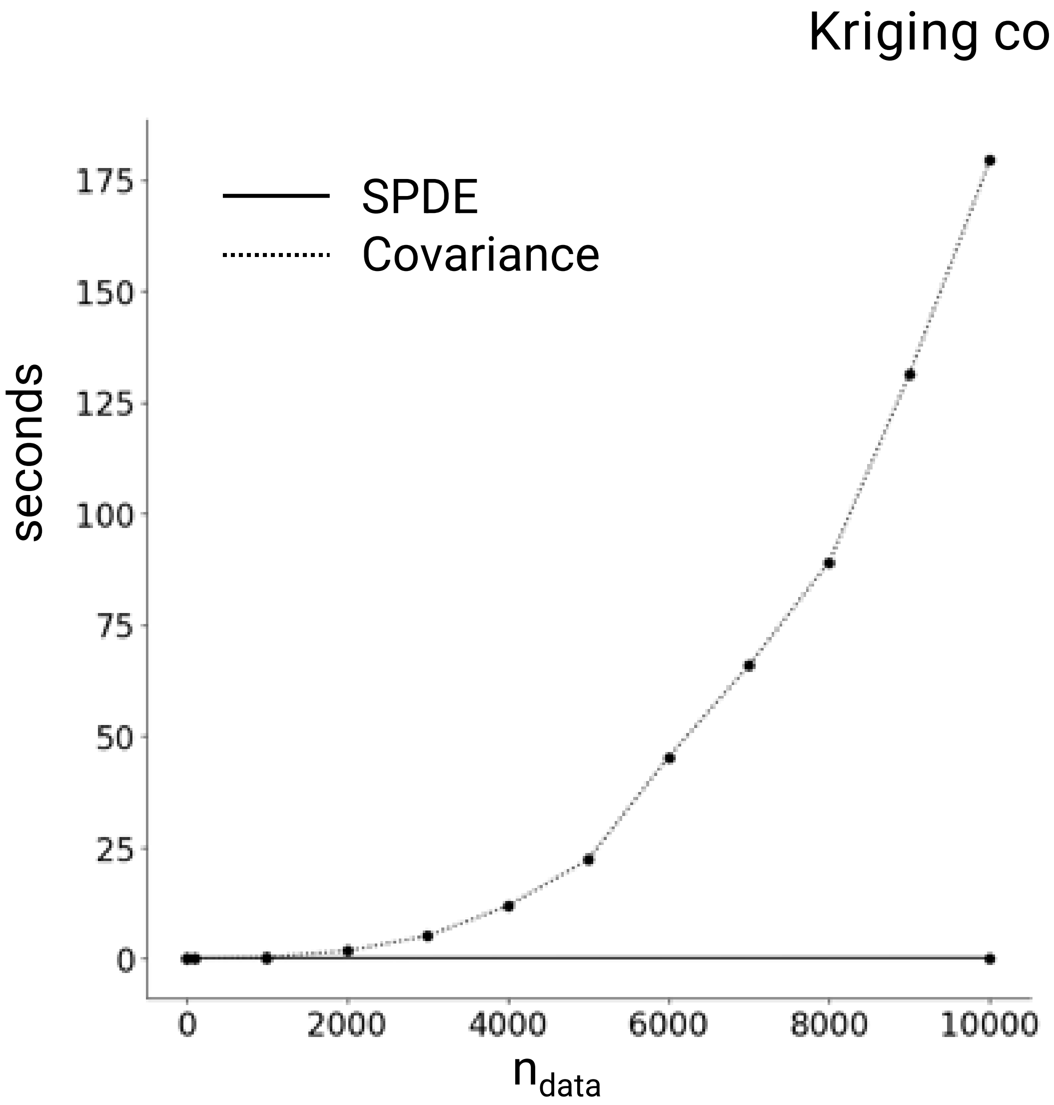
Computation times benchmark

Number of data, SPDE approach vs covariance approach

Underlying mesh resolution

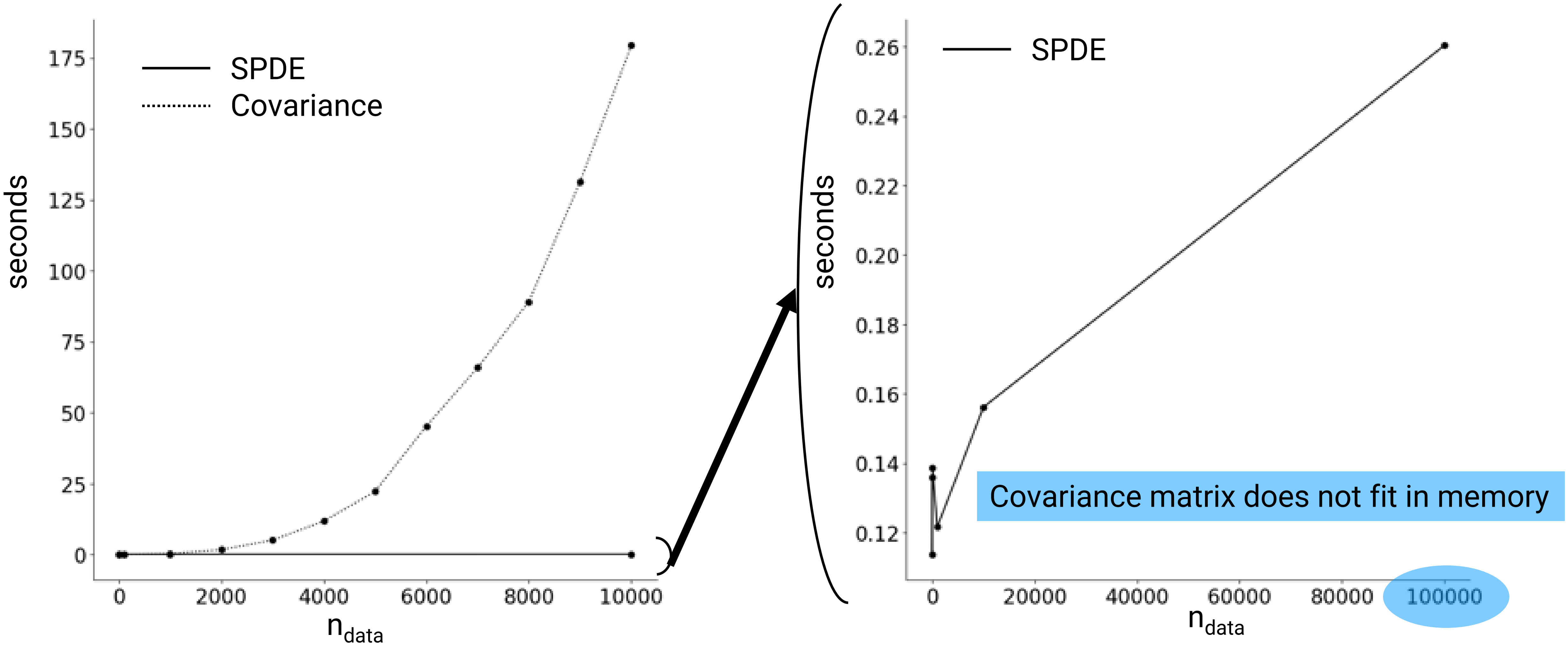
Smoothness param ν

Computation times benchmark, SPDE vs covariance



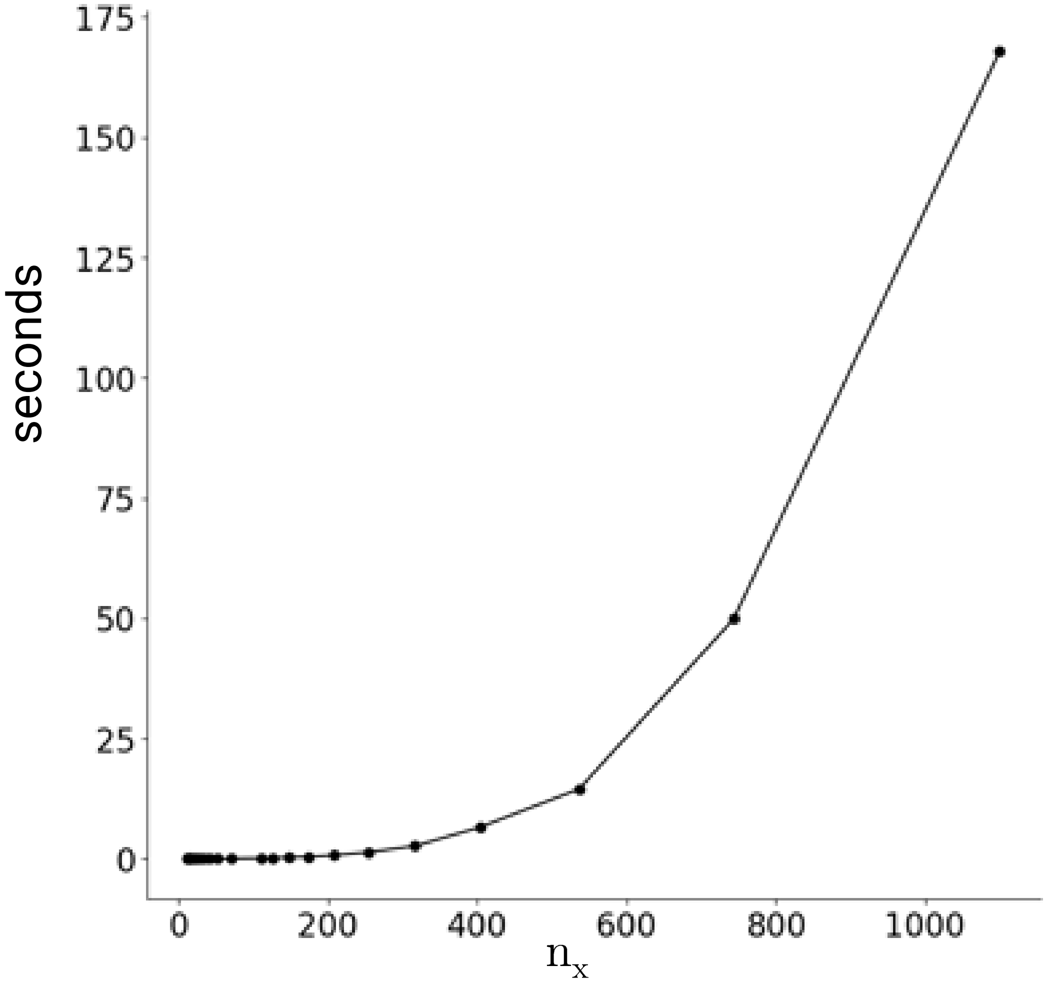
Computation times benchmark, SPDE vs covariance

Kriging computation time



Covariance matrix does not fit in memory

Computation times benchmark, underlying mesh

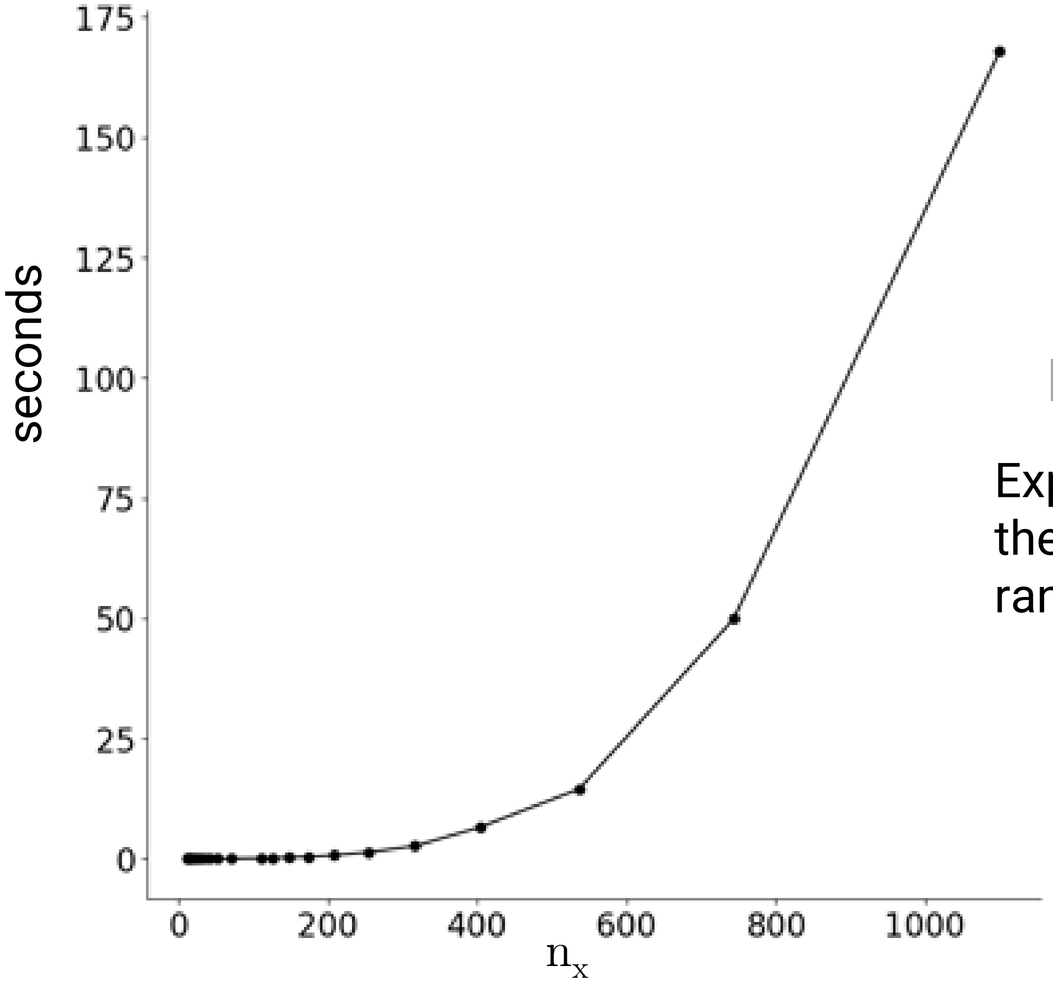


Kriging computation time

Underlying mesh resolution $n_x \times n_x$

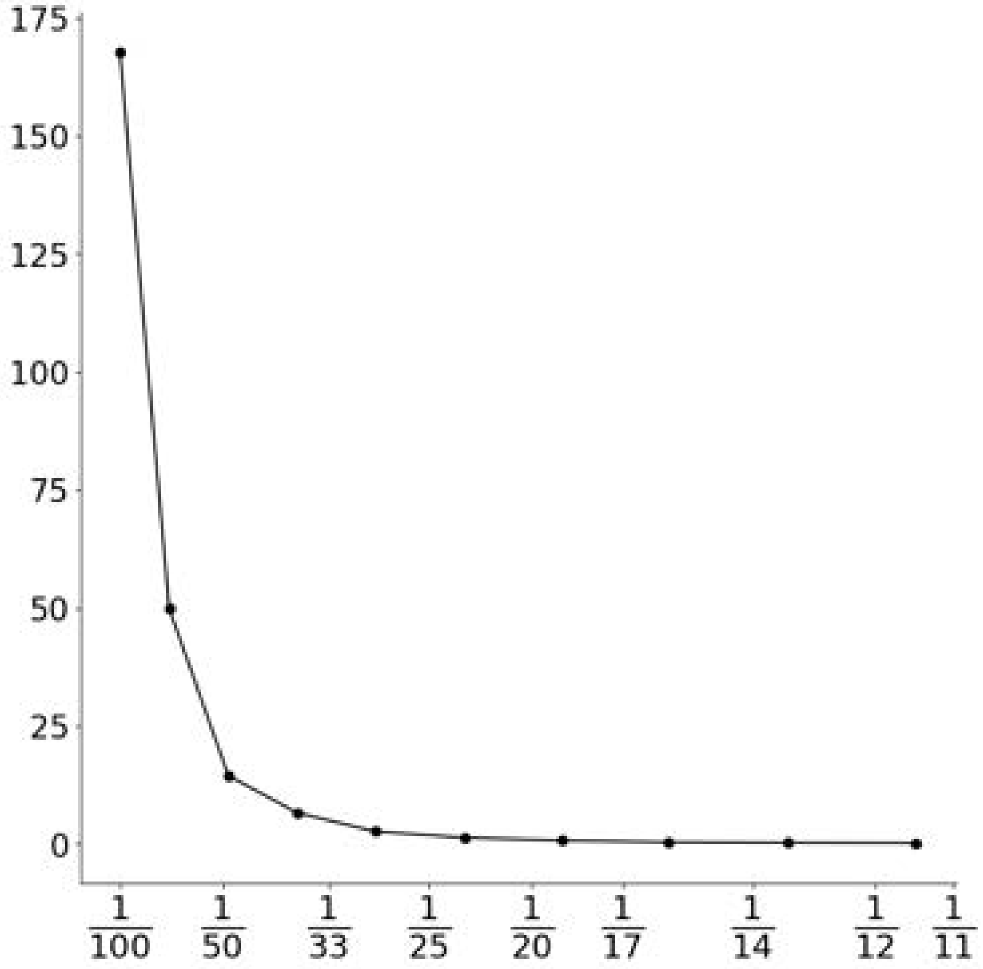
Computation times benchmark, underlying mesh

Kriging computation time



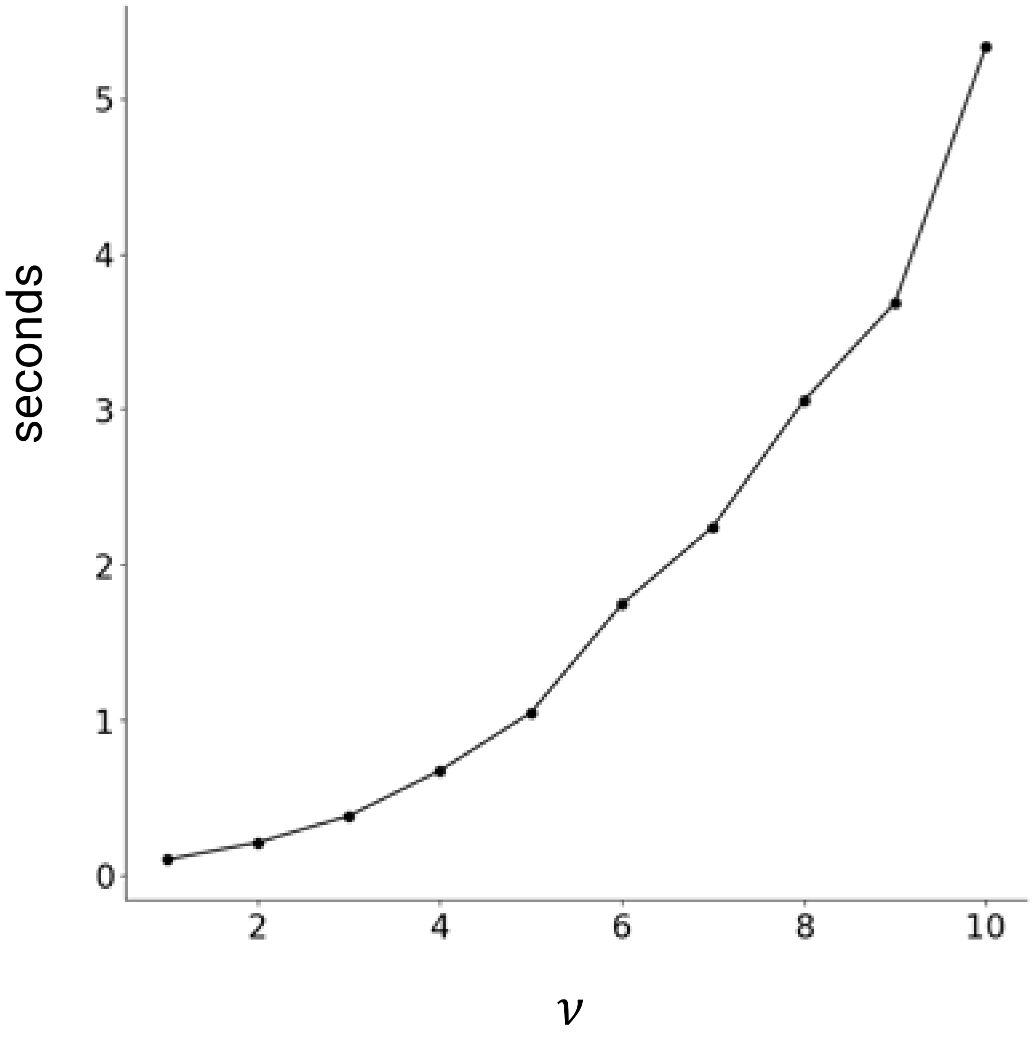
Underlying mesh resolution $n_x \times n_x$

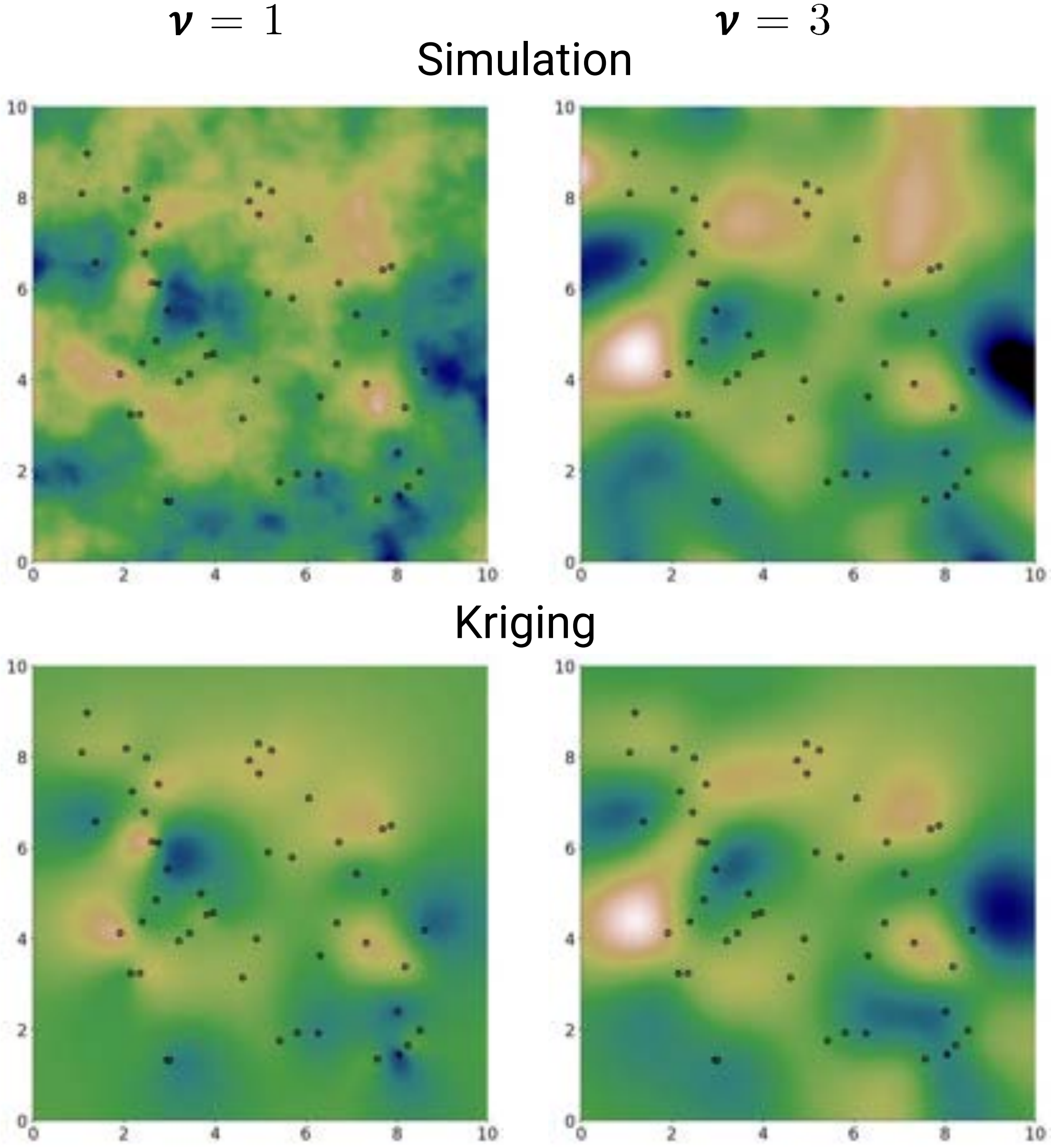
Expressed with the variogram range



Ratio $\frac{range}{domain\ size}$

Computation times benchmark, smoothness param ν




$\nu = 1$

$\nu = 3$

Simulation

Kriging

To summarize

- The SPDE approach allows to compute GRF
- Computation times:
  - is independent of the amount of data
  - decrease when the variogram range of the GRF increase
  - increase when the smoothness of the GRF increase

➔ SPDE approach is faster than the covariance approach

To summarize

- The SPDE approach allows to compute GRF
- Computation times:
  - is independent of the amount of data
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➔ SPDE approach is faster than the covariance approach

- Let’s go back to

How are uncertainties taken into account in the SPDE process?

Data uncertainties with the SPDE

- Assumption: data are coming from a GRF with a measurement noise

→ $\mathrm{Y}_{\mathrm{data}} = \mathrm{A}\mathrm{Z}_{\mathrm{GRF}} + \varepsilon$

A: mask matrix, ε: Gaussian noise with variance σ^2

Data uncertainties with the SPDE

- Assumption: data are coming from a GRF with a measurement noise

→ $\mathrm{Y}_{\mathrm{data}} = \mathrm{AZ}_{\mathrm{GRF}} + \varepsilon$

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- Due to this measurement noise/assumption, the conditioning is not exact*

*however, post-processing is possible for exact conditioning

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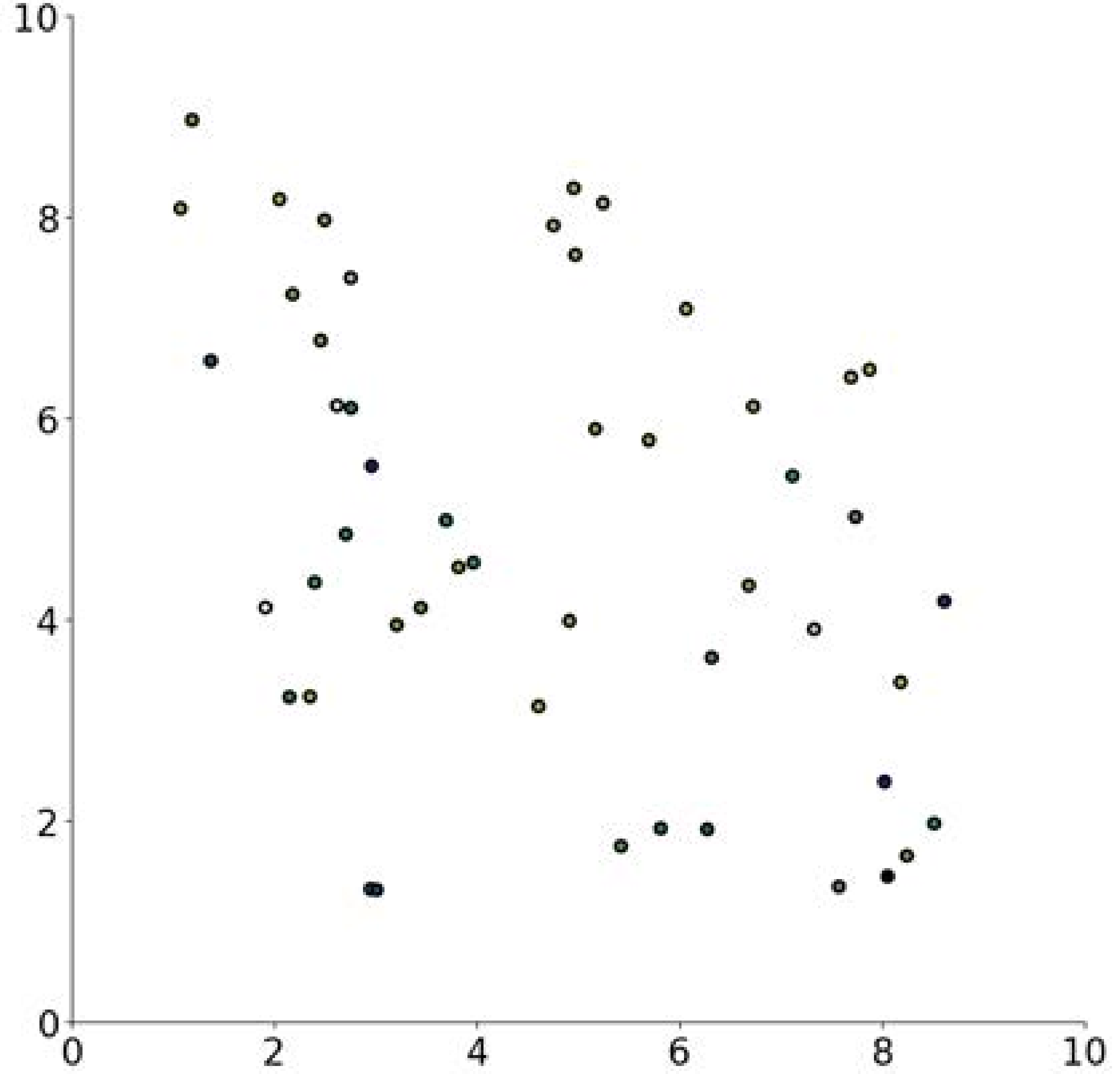
*however, post-processing is possible for exact conditioning

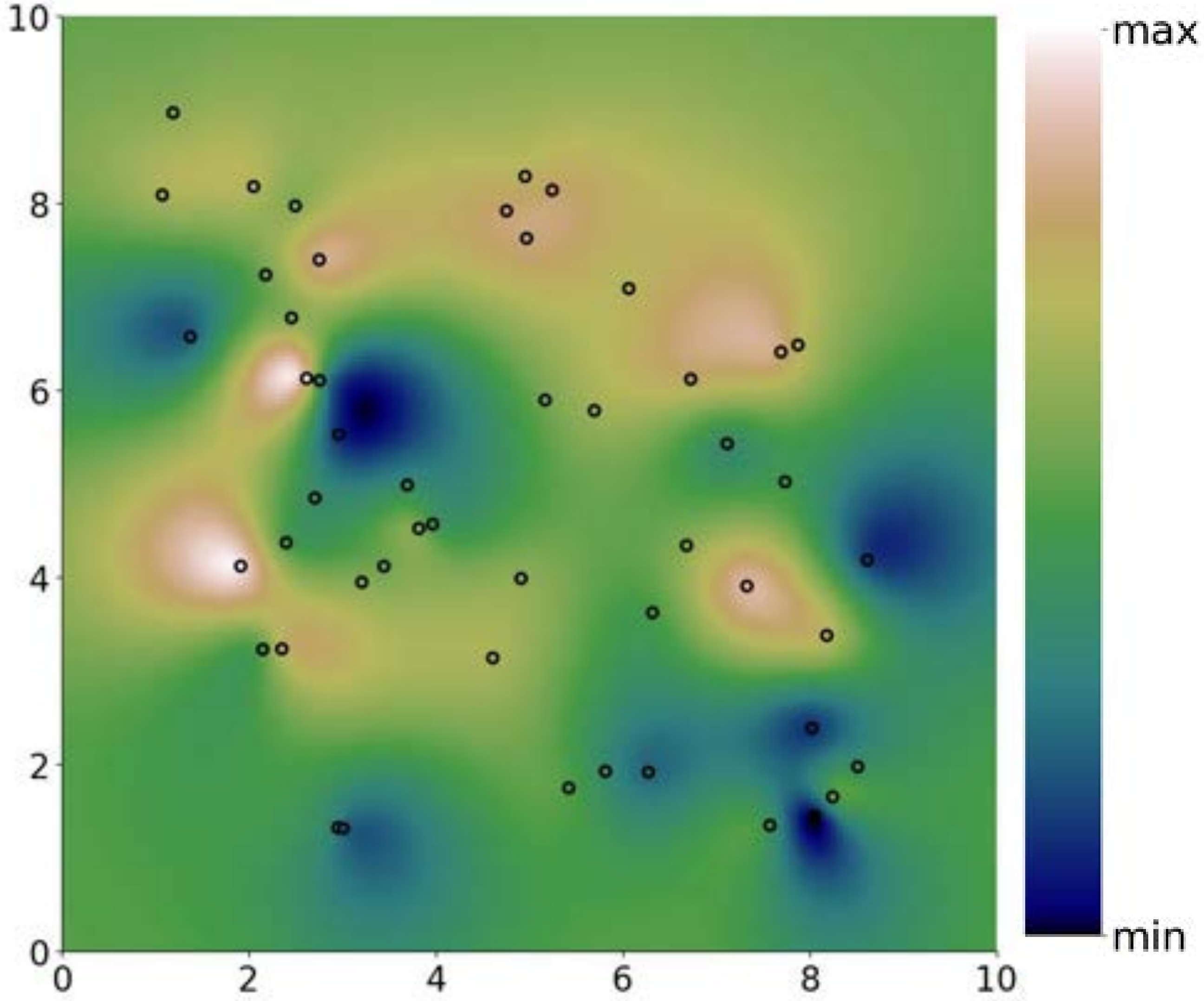
- Simulations are fast to compute, allowing to access uncertainties
- The simulations mean is the kriging

The kriging with SPDE

Conditioning data, *e.g.* altitude measurement

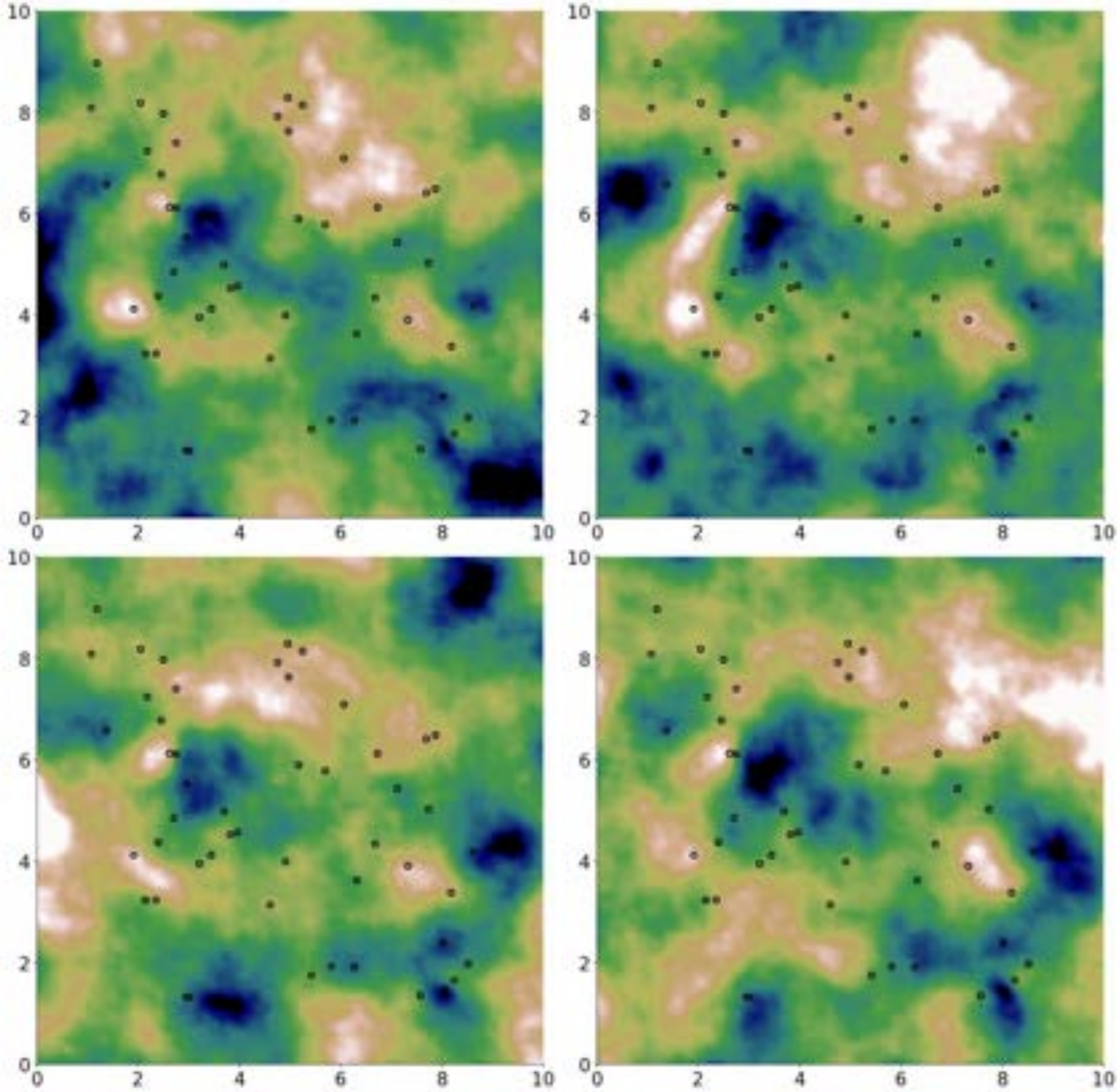


Kriging (simulations means)



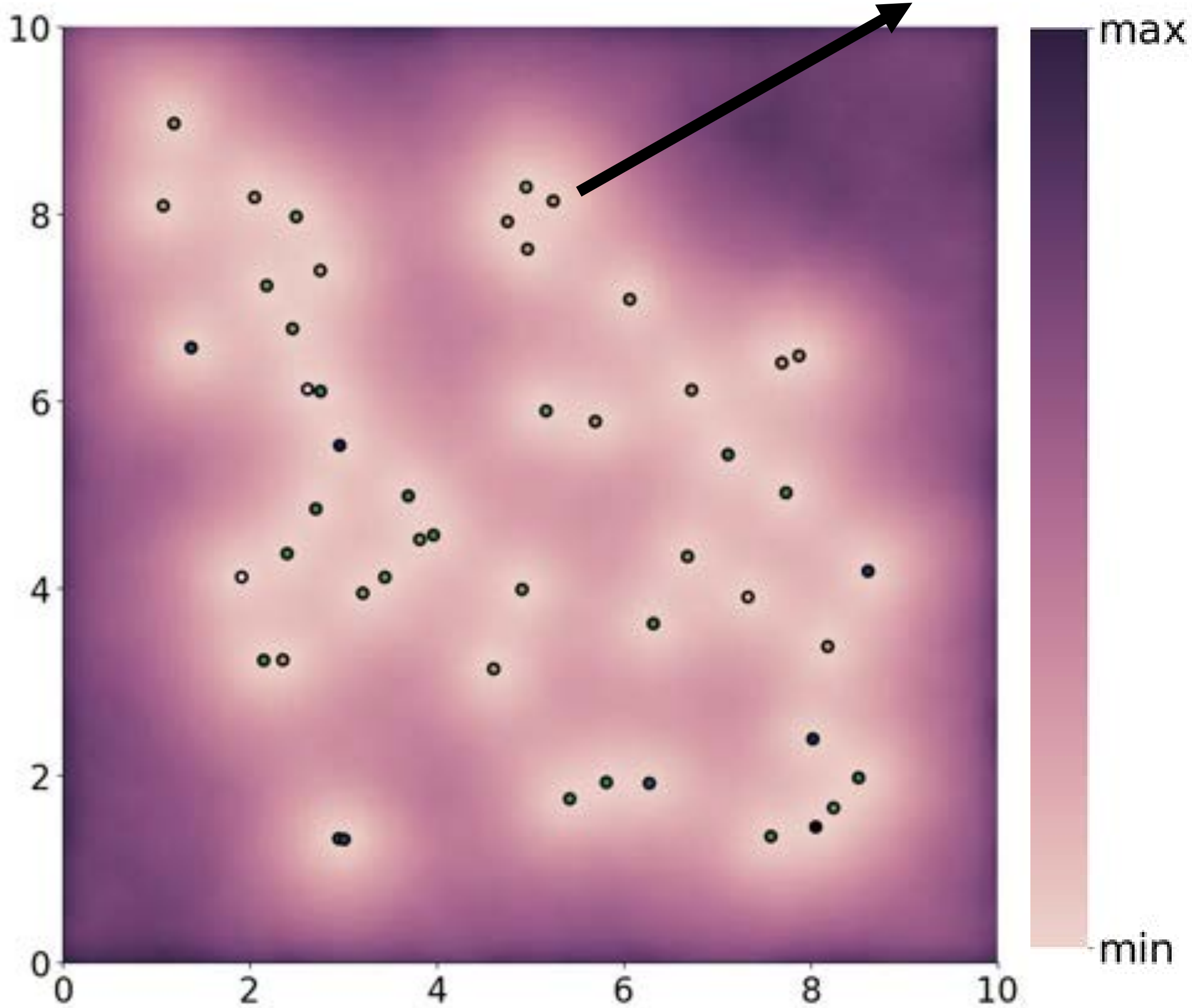
Conditional simulations with SPDE

4 conditional simulations



Variance

Increase with the distance with data



Ongoing work

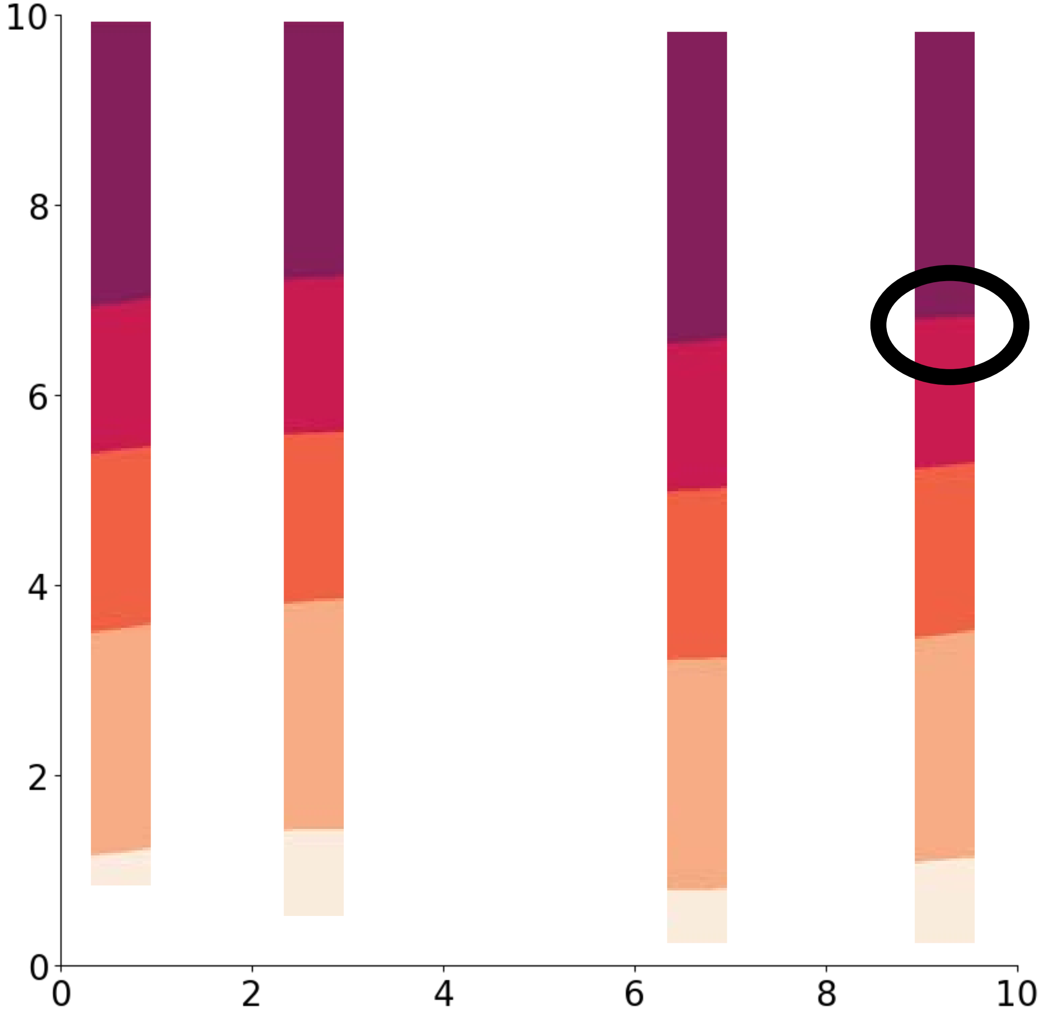
Geological modeling with SPDE, based on the potential field method (Lajaunie et al., 1997)

Inequality data $\mathrm{Z}(\mathrm{x}) \in [\mathrm{A},\, \mathrm{B}]$, based on Gibbs sampling (Freulon, 1992)

SPDE kriging and simulations with a fault (based on the work of Marechal, 1984)

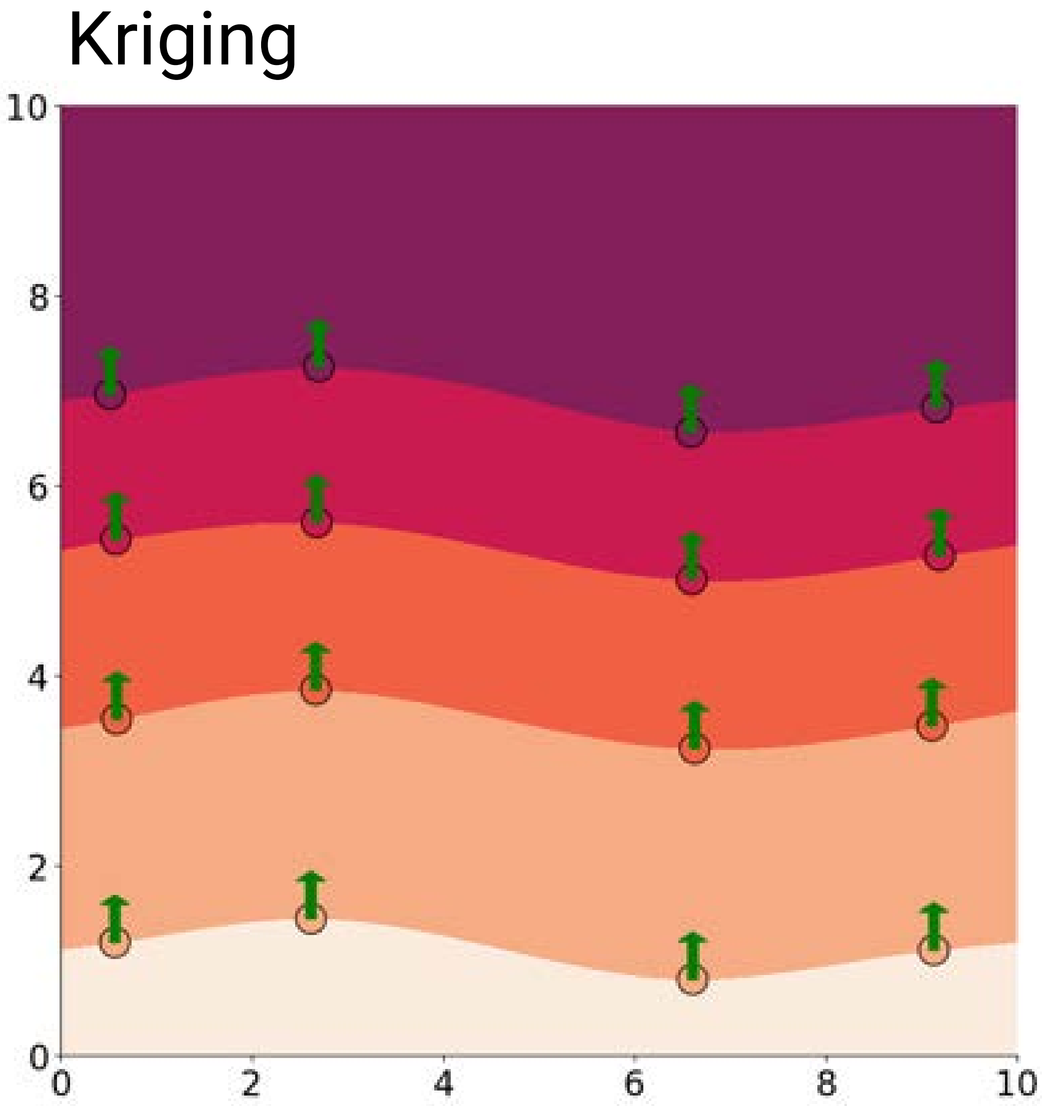
Geological modeling with SPDE, based on the potential field method

Drillholes data



Only interfaces will be taken into account

Geological modeling with SPDE, based on the potential field method



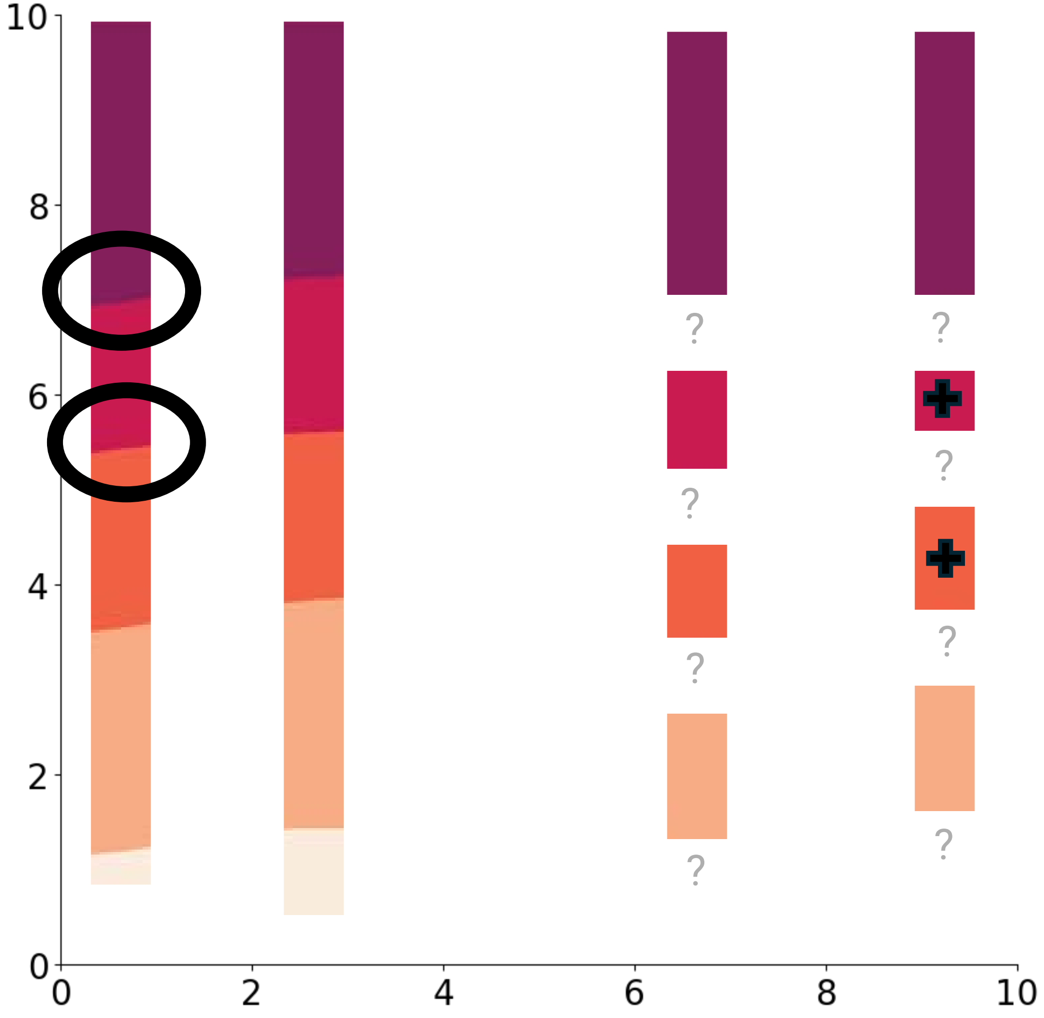
● Interface

⬆ Younging direction

Inequality data, based on Gibbs sampling

Drillholes data with missing interfaces

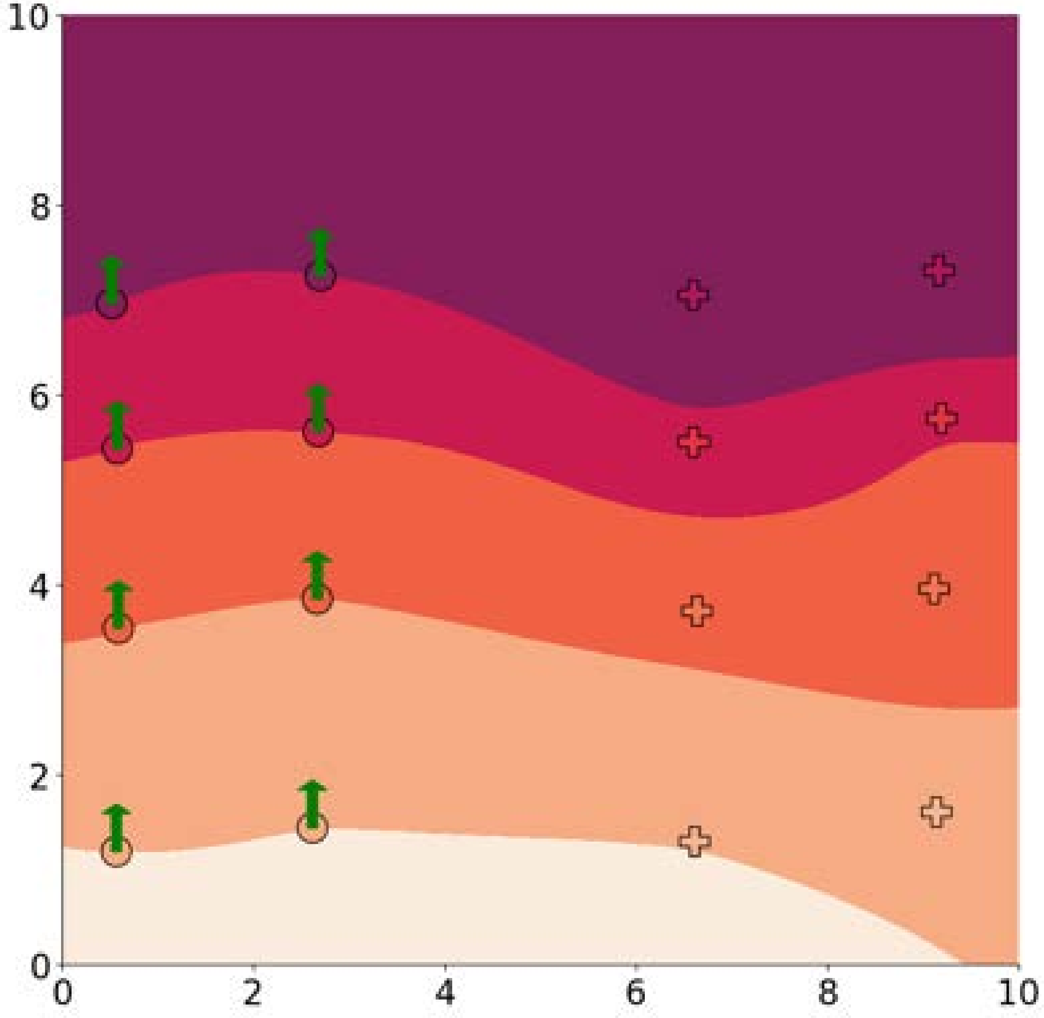
Here interfaces will be taken into account



- Here, interfaces are not observed
- But we have information of points between two interfaces "$\mathrm{Z(x)} \in [\mathrm{A},\ \mathrm{B}]$"

Inequality data, based on Gibbs sampling

Kriging with inequality



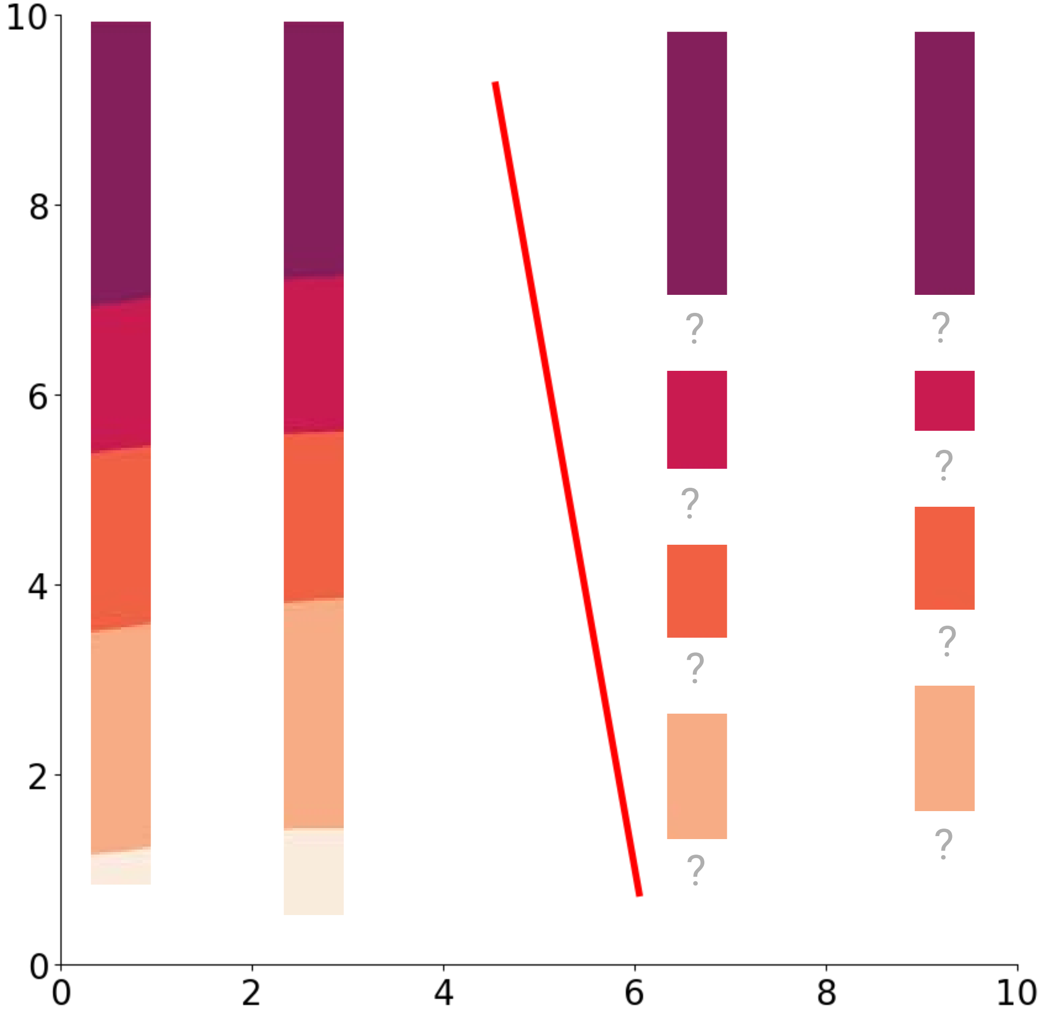
● Interface

⬆ Younging direction

✚ Point between
two interfaces
“Inequality constraint”

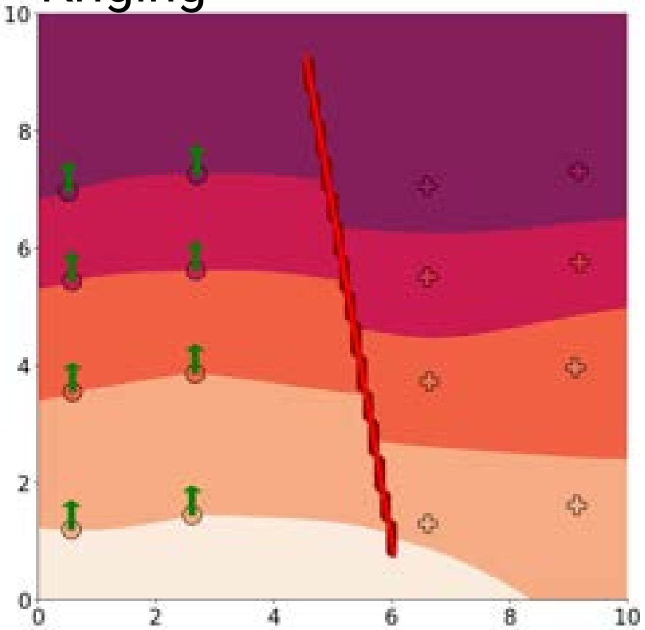
What happens when there is a geological fault?

Drillholes data with a known fault



Kriging and simulations with a fault

Kriging

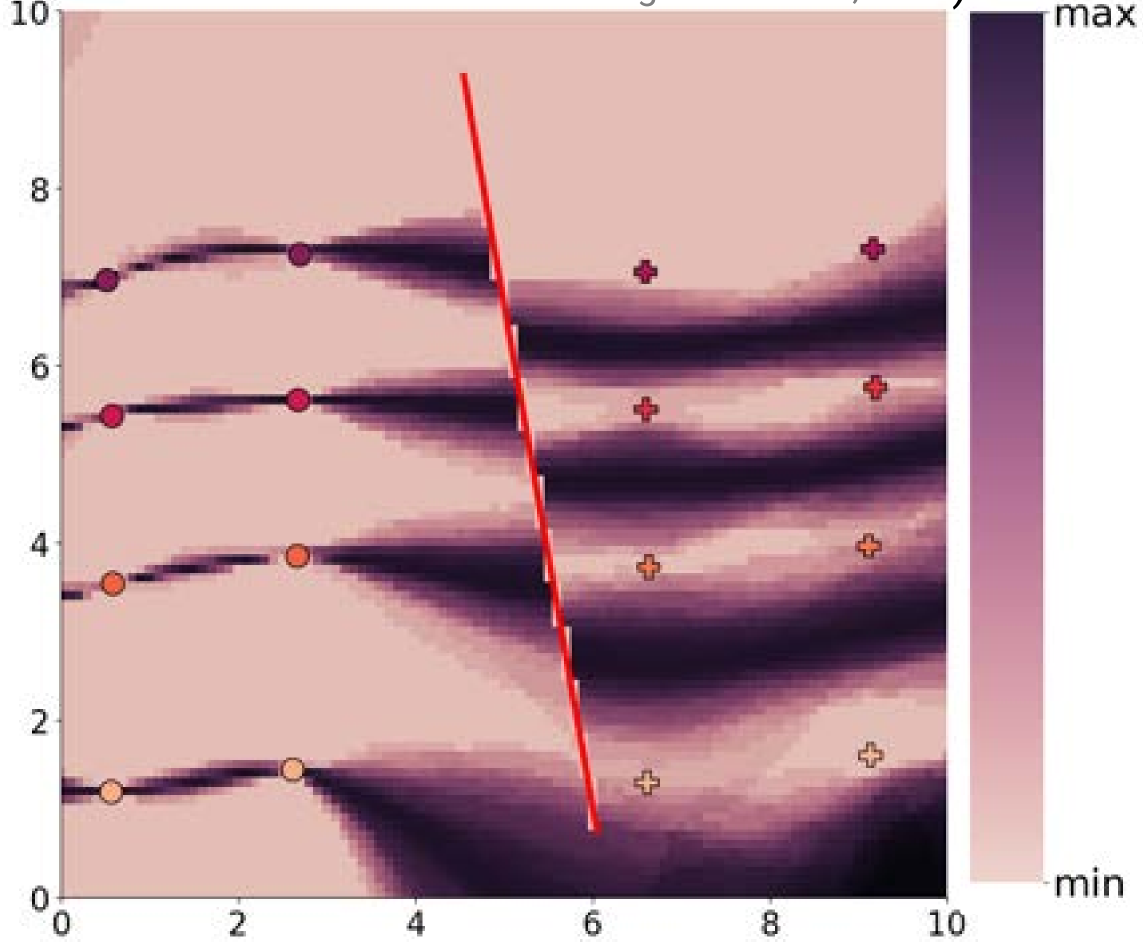


● Interface

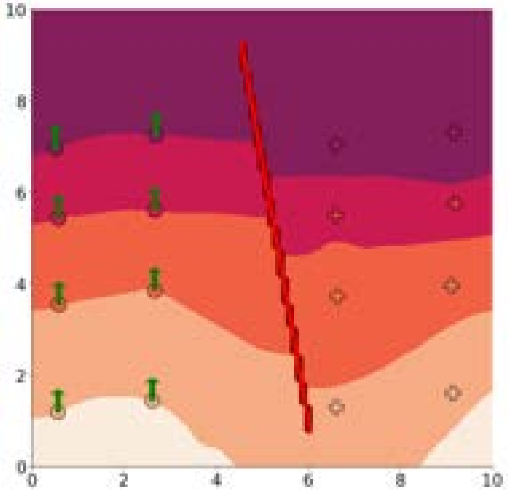
⬆ Younging direction

✚ Point between two interfaces “Inequality constraint”

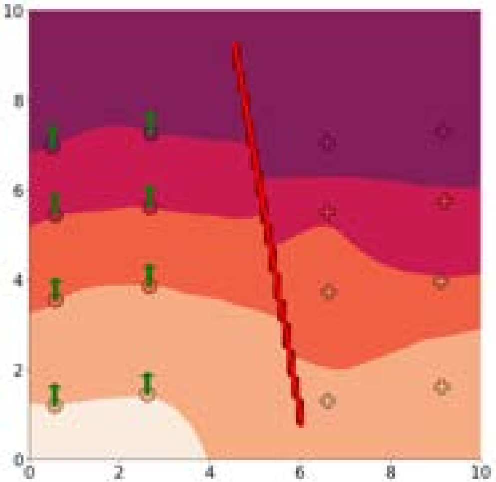
Uncertainty map (Shannon entropy, Wellmann and Regenauer-Lieb, 2012)



Simulation 1



Simulation 2



Conclusion

- The SPDE approach is an alternative of the “classic” covariance approach for geostatistics
- The SPDE approach is faster, and computation time don’t depend on the amount of data

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- The SPDE approach is faster, and computation time don’t depend on the amount of data

- Ongoing works to be able to:
  - Use SPDE for geological modeling
  - Use inequality constraints with SPDE
  - Take into account the presence of faults

Conclusion

- The SPDE approach is an alternative of the “classic” covariance approach for geostatistics
- The SPDE approach is faster, and computation time don’t depend on the amount of data

- Ongoing works to be able to:
    - Use SPDE for geological modeling
    - Use inequality constraints with SPDE
    - Take into account the presence of faults

- Computations done with the open-source library gstlearn (C++, R, python)

github.com/gstlearn/gstlearn

Thank you for your attention!

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