GeoBlocks: Building blocks for the quantification of uncertainties in geological models

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24.10.2023

URS2023

Outline

- Recapitulation
- Work Progress
- Input Data and Implicit Model with GemPy
- Object-Distance Simulation (ODSIM) Approach
- Probabilistic Uncertainty Approach
- Discussion
- Next Steps

Recapitulation

- Data Management Plan (DMP) (ongoing)
- GIS Database (started)
- Revision of explicit and implicit geomodelling methods (ongoing)
- Model building with GemPy (ongoing)

Work Progress

Gaussian Process Application

Coordinates & Orientation → **GemPy Model** → **ODSIM Approach** → **Spatial Uncertainty Quantification** → **Uncertainty Reduction**

Seismic Borehole data | Large-scale features | Small-scale features

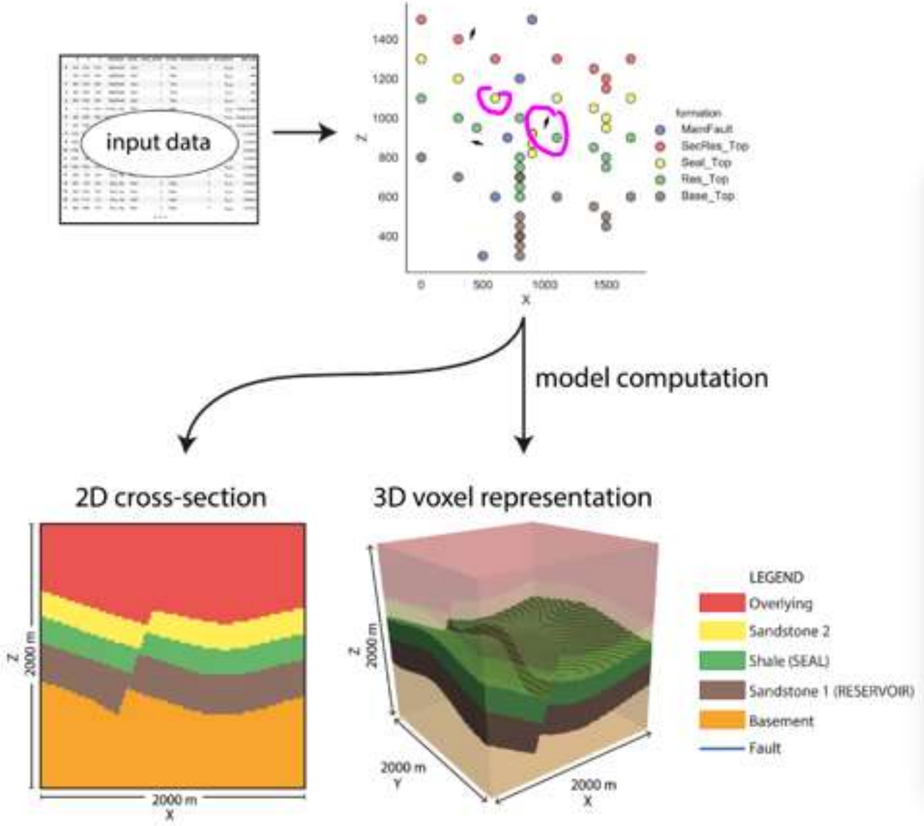
Current work

GemPy: Miguel de la Varga and J. Florian Wellmann. 2016. Structural geologic modeling as an inference problem: A Bayesian perspective. Interpretation 2016; 4 (3): SM1–SM16.
ODSIM: Vincent Henrion, Guillaume Caumon and Nicolas Cherpeau. 2010. ODSIM: An Object-Distance Simulation Method for Conditioning Complex Natural Structures. International Association for Mathematical Geosciences.

GeoBlocks Project Goal

To provide a workflow to quantify and minimize uncertainties for the selection of a storage site in Germany for nuclear waste

Input Data and Implicit Model with GemPy

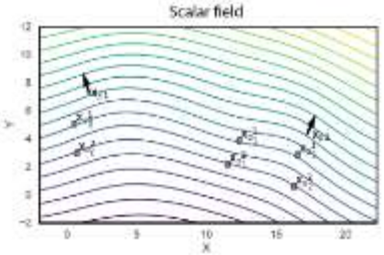


https://docs.gempy.org
De la Varga M., Schaaf A., and Wellmann F. (2019)
Wellmann F. (n. d.)

Interpolation function $\mathbf{Z}(\boldsymbol{x}_0), (x, y, z) \in \mathbb{R}^3$

Gradient of the scalar field follows the planar orientation

Interfaces as isosurfaces



Characterisation of the scalar field:
interface points $\boldsymbol{x}_0$
gradients of scalar field $\boldsymbol{x}_\alpha$

Universal cokriging **Chiles and Delfiner (2009)**

$$\begin{bmatrix} \mathbf{C}_{\partial Z/\partial u,\, \partial Z/\partial v} & \mathbf{C}_{\partial Z/\partial u,\, Z} & \mathbf{U}_{\partial Z/\partial u} \\ \mathbf{C}_{Z,\, \partial Z/\partial u} & \mathbf{C}_{Z,\, Z} & \mathbf{U}_{Z} \\ \mathbf{U}'_{\partial Z/\partial u} & \mathbf{U}'_{Z} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \boldsymbol{\lambda}_{\partial Z/\partial u,\, \partial Z/\partial v} & \boldsymbol{\lambda}_{\partial Z/\partial u,\, Z} \\ \boldsymbol{\lambda}_{Z,\, \partial Z/\partial u} & \boldsymbol{\lambda}_{Z,\, Z} \\ \boldsymbol{\mu}_{\partial u} & \boldsymbol{\mu}_{u} \end{bmatrix} = \begin{bmatrix} \mathbf{c}_{\partial Z/\partial u,\, \partial Z/\partial v} & \mathbf{c}_{\partial Z/\partial u,\, Z} \\ \mathbf{c}_{Z,\, \partial Z/\partial u} & \mathbf{c}_{Z,\, Z} \\ \boldsymbol{f}_{10} & \boldsymbol{f}_{20} \end{bmatrix}$$

De la Varga M., Schaaf A., and Wellmann F. (2019)

GemPy

Input Data and Implicit Model with GemPy

NURBS

Parametric 3D surfaces

(explicit model definition)

Higher order basis functions interpolating a control network of surface nodes

Wellmann F. and Caumon (2018)

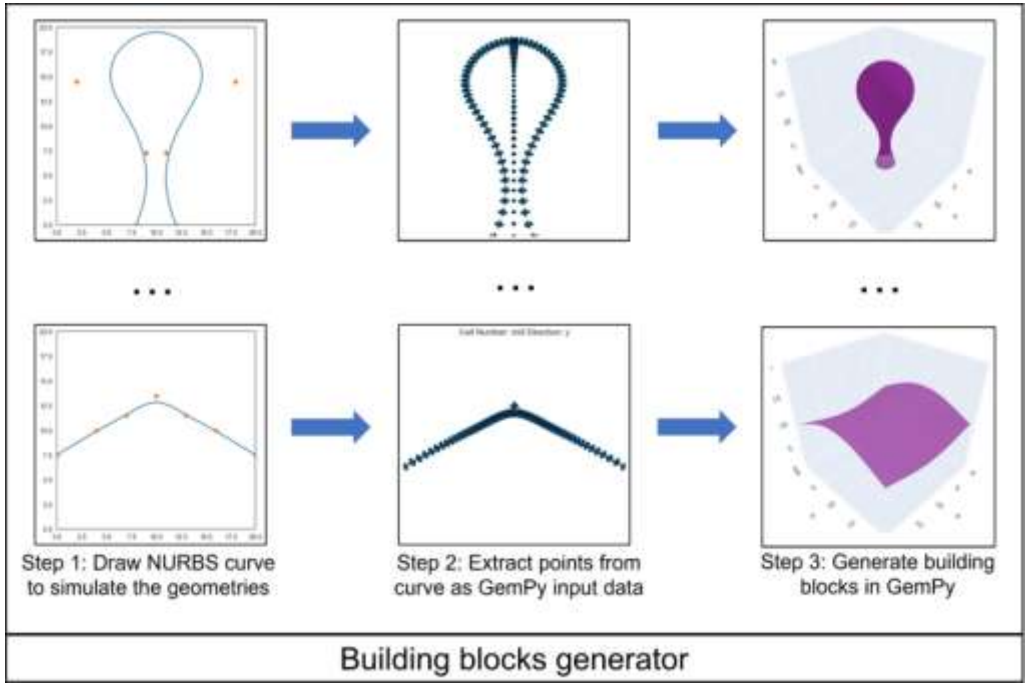
GemPy

Implicit modelling

Universal cokriging interpolation

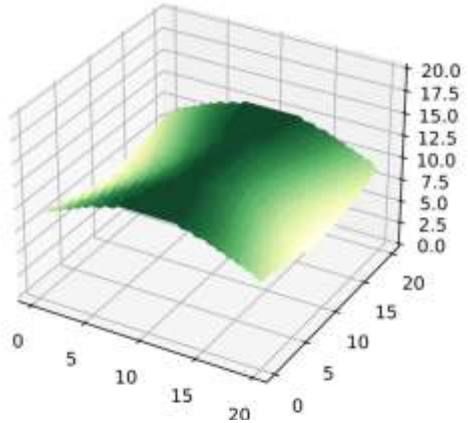
https://docs.gempy.org

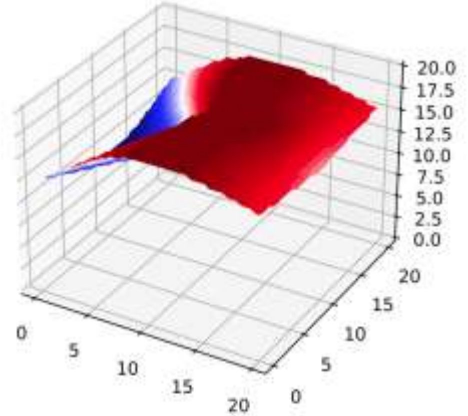
De la Varga M., Schaaf A., and Wellmann F. (2019)



Yang et al. (2023)

3D Grid





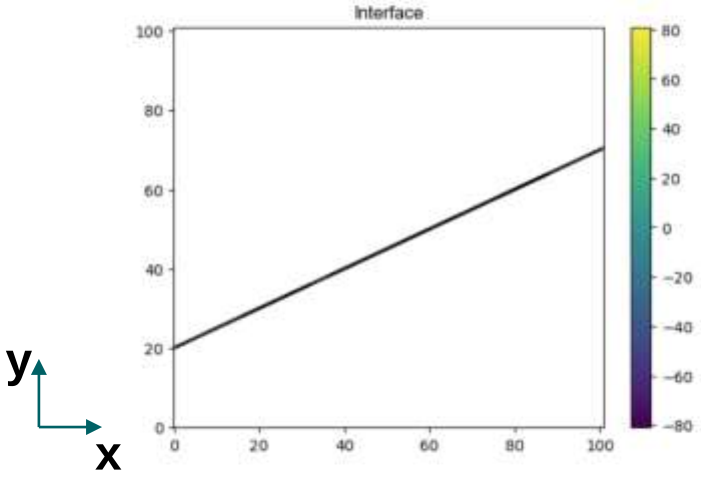
DATA

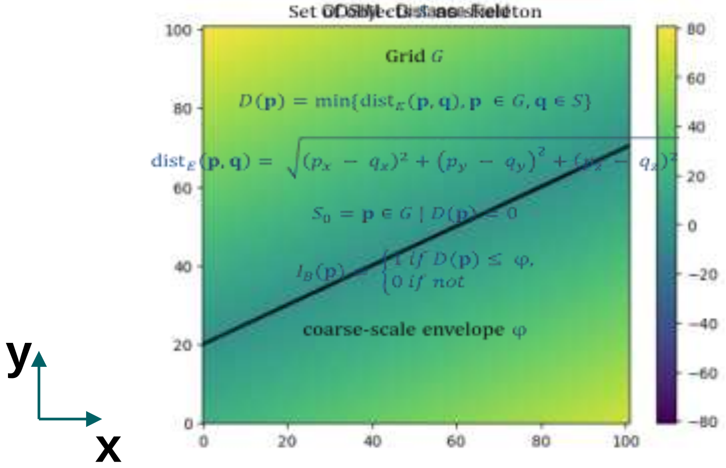
Synthetic Standard Model

Simulated Observed Data

Python Programming language | GemPy | PyMC3 | NumPy | matplotlib

Object-Distance Simulation (ODSIM) Approach





Modified from Henrion et al., 2010

Set of objects S as skeleton

Grid G

$$D(\mathbf{p}) = \min\{\text{dist}_E(\mathbf{p},\mathbf{q}), \mathbf{p} \in G, \mathbf{q} \in S\}$$

$$\text{dist}_E(\mathbf{p},\mathbf{q}) = \sqrt{(p_x - q_x)^2 + \left(p_y - q_y\right)^2 + (p_z - q_z)^2}$$

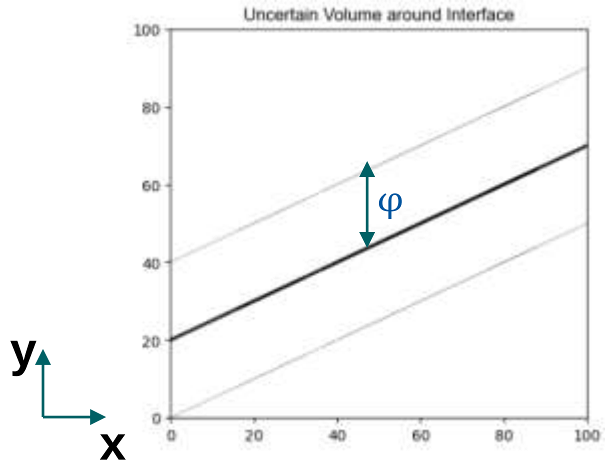
$$S_0 = \mathbf{p} \in G \mid D(\mathbf{p}) = 0$$

$$I_B(\mathbf{p}) = \begin{cases} 1 \; if \; D(\mathbf{p}) \leq \varphi, \\ 0 \; if \; not \end{cases}$$

coarse-scale envelope φ

Henrion et al., 2010

$$\varphi \sim \text{Uniform}\,(b_1, b_2)$$



We consider our synthetic geological model as the ODSIM skeleton.

Then, a random distance from the skeleton (sampled from a uniform distribution) becomes the mean for the Gaussian surface.

Probabilistic Uncertainty Approach

MEAN OF GAUSSIAN SURFACE

$\mu_{gf} \sim \text{Uniform}\,(b_1, b_2)$

COVARIANCE (Squared Exponential)

$Cov = e^{-\frac{r^2}{2l^2}}$

GAUSSIAN SURFACE

$Gaussian\ feature \sim \text{Mult. Normal}\,(\mu_{gf}, Cov)$

VARIANCE OF GAUSSIAN SURFACE

$\sigma_{gf} \sim \text{Uniform}\,(s_1, s_2)$

VARIANCE OF DATA

$\sigma_d \sim \text{Uniform}\,(d_1, d_2)$

DATA

PRIOR

GAUSSIAN SURFACE

+

SYNTHETIC STANDARD MODEL

$Prior \sim \text{Normal}\,(\mu_p, \sigma_{gf})$

LIKELIHOOD

Observed data

$Likelihood \sim \text{Normal}\,(data, \sigma_d)$

POSTERIOR

Final Model

The goal of the approach is to sample a random model or surface in the proximity of the synthetic standard geological model, to later condition it to the observed data, while simultaneously incorporating the uncertainty of both the method and data.

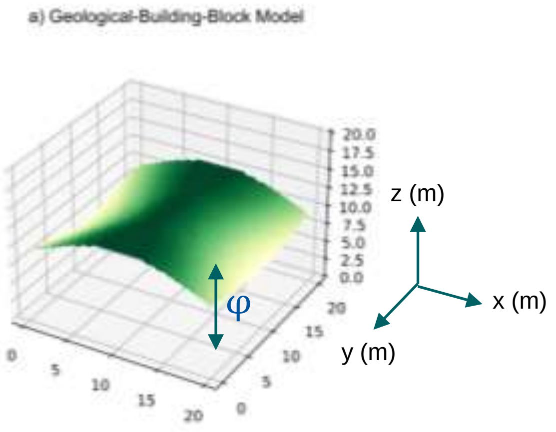
Python Programming language

PyMC3

NumPy

Probabilistic Uncertainty Approach

a) Incorporate synthetic geological model



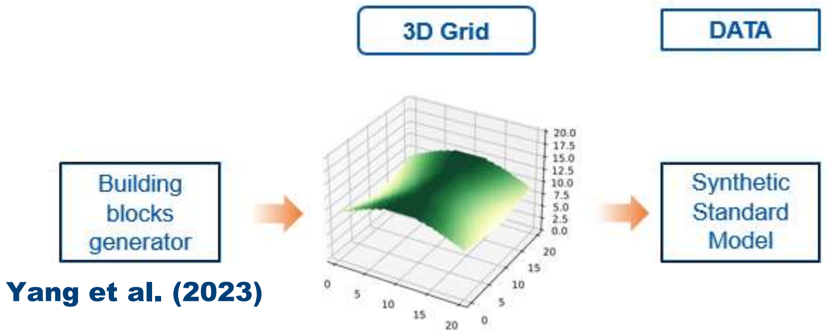
Synthetic standard geological model = skeleton

Uncertainty in the vertical direction, sampled from a uniform distribution

$$\varphi = \mu_{gf} \sim \text{Uniform}\ (-5, 5)$$

This distance becomes the mean of the Gaussian surface of next step

The limits of the uniform distribution expect to address the uncertainties given by the area where the synthetic geological model is applied

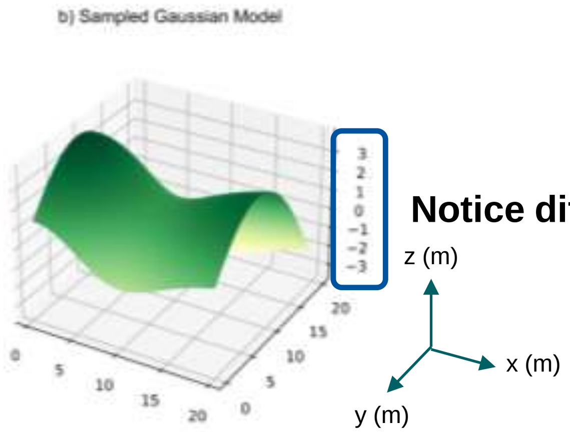


Python Programming language · GemPy · PyMC3 · NumPy · matplotlib

Probabilistic Uncertainty Approach

a) **Incorporate synthetic geological model**

Colour bars



Notice different scale

b) **Create Gaussian surface within the uncertain volume**

With the mean of previous step, we create a Gaussian surface with the following parameters:

$$\mu_{gf} \sim \text{Uniform}\ (-5, 5)$$

Stationary Covariance Functions:

$\boxed{\text{Squared Exponential}}$

The Matérn Class

Ornstein-Uhlenbeck Process and Exponential

γ-exponential

Rational Quadratic

Piecewise Polynomial

Dot Product Covariance Functions

Non-stationary Covariance Functions

Universal

Discontinuities not expected

Non periodic model

Smooth

$$Cov = e^{-\frac{r^2}{2l^2}}$$

$$\text{with l} = 10\ \text{m} \ll 100\ \text{m}$$

Rasmussen and Williams, 2006
Duvenaud, 2014

$$Gaussian\ feature \sim \text{Mult. Normal}\ (\mu_{gf}, Cov)$$

Python Programming language GemPy PyMC3 NumPy matplotlib

Probabilistic Uncertainty Approach

a) **Incorporate synthetic geological model**

b) **Create Gaussian surface within the uncertain volume**

$$Gaussian\ feature \sim \text{Mult. Normal}\ (\mu_{gf}, Cov)$$

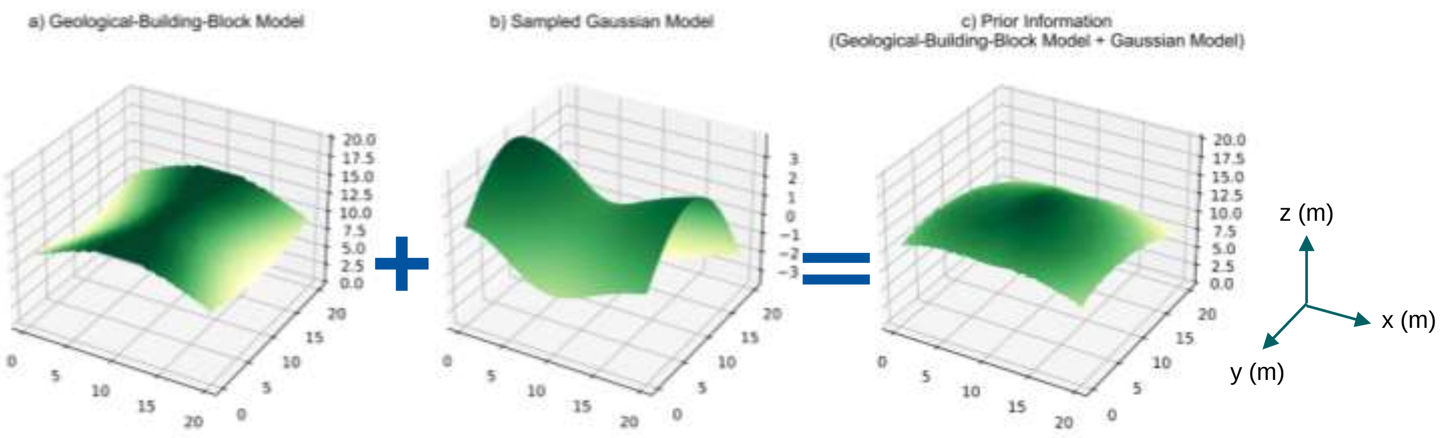
$$\sigma_{gf} \sim \text{Uniform}\ (-1, 1)$$

c) **Add previous surfaces to get the mean of the prior model**

The sum of the surfaces obtained in steps a) and b) become the mean of a normal distribution for the prior model

$$\mu_p = Synthetic\ Geological\ Model + Gaussian\ feature$$

$$Prior \sim \text{Normal}\ (\mu_p, \sigma_{gf})$$



Prior

Python
Programming language
GemPy
PyMC3
NumPy
matplotlib

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Computational Geoscience and Reservoir Engineering

RWTH AACHEN UNIVERSITY

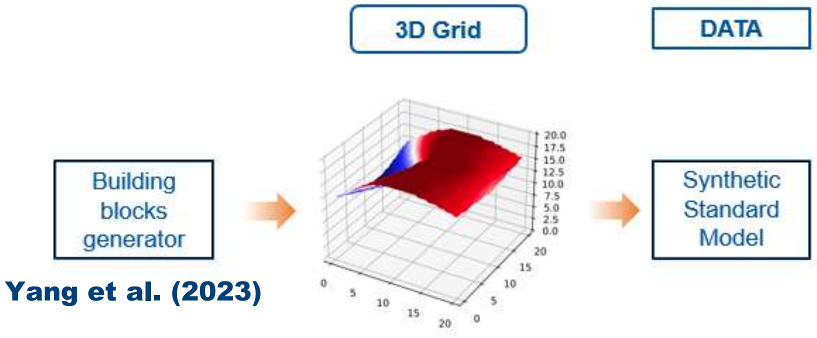
Probabilistic Uncertainty Approach

a) Incorporate synthetic geological model

b) Create Gaussian surface within the uncertain volume

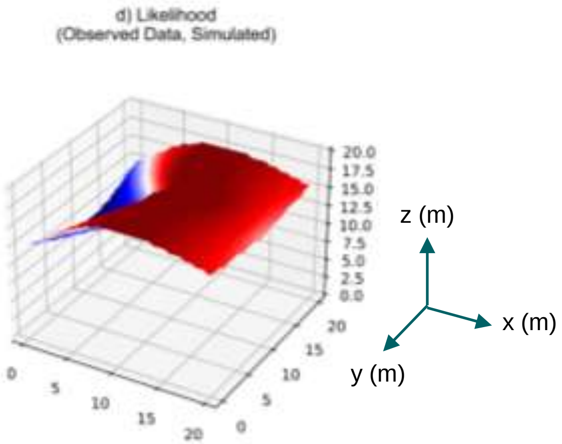
c) Add previous surfaces to get the mean of the prior model

d) Incorporate observations as likelihood



Based on De la Varga M. and Wellmann J. F. (2016), we incorporate the observations as the likelihood function.

The variance of the normal distribution that expects to address the uncertainty of the observations.



$$Likelihood \sim \text{Normal}\,(data, \sigma_d)$$

Python Programming language GemPy PyMC3 NumPy matplotlib

URS2023

Computational Geoscience and Reservoir Engineering

RWTH AACHEN UNIVERSITY

Probabilistic Uncertainty Approach

a) Incorporate synthetic geological model

b) Create Gaussian surface within the uncertain volume

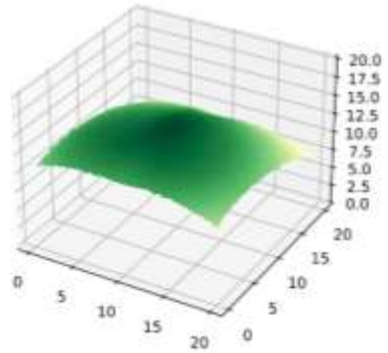
c) Add previous surfaces to get the mean of the prior model

d) Incorporate observations as likelihood

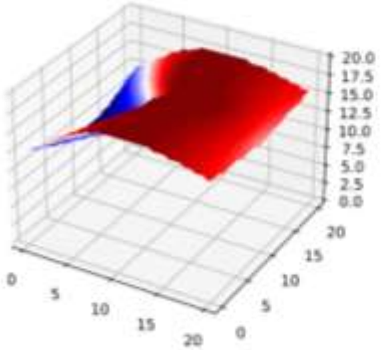
e) Predict adaptation, posterior model

We get the posterior model from previously obtained prior model on likelihood function

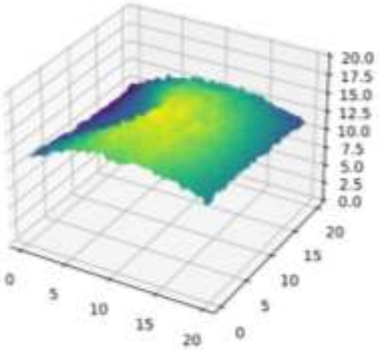
c) Prior Information
(Geological-Building-Block Model + Gaussian Model)



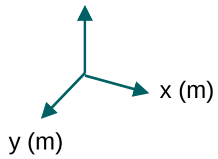
d) Likelihood
(Observed Data, Simulated)



e) Posterior Model
(Final Model)



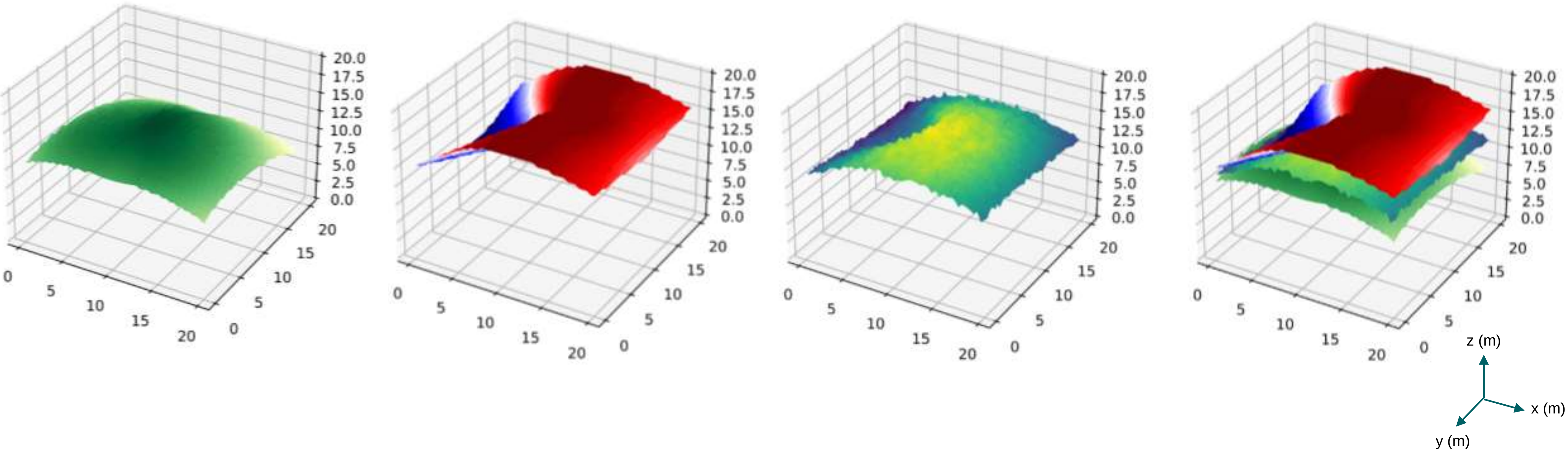
Posterior



Python Programming language   GemPy   PyMC3   NumPy   matplotlib

Probabilistic Uncertainty Approach

Prior *Likelihood (Observations)* *Posterior* *All*



Python
GemPy
PyMC3
NumPy
matplotlib

Probabilistic Uncertainty Approach

a) **Incorporate synthetic geological model**

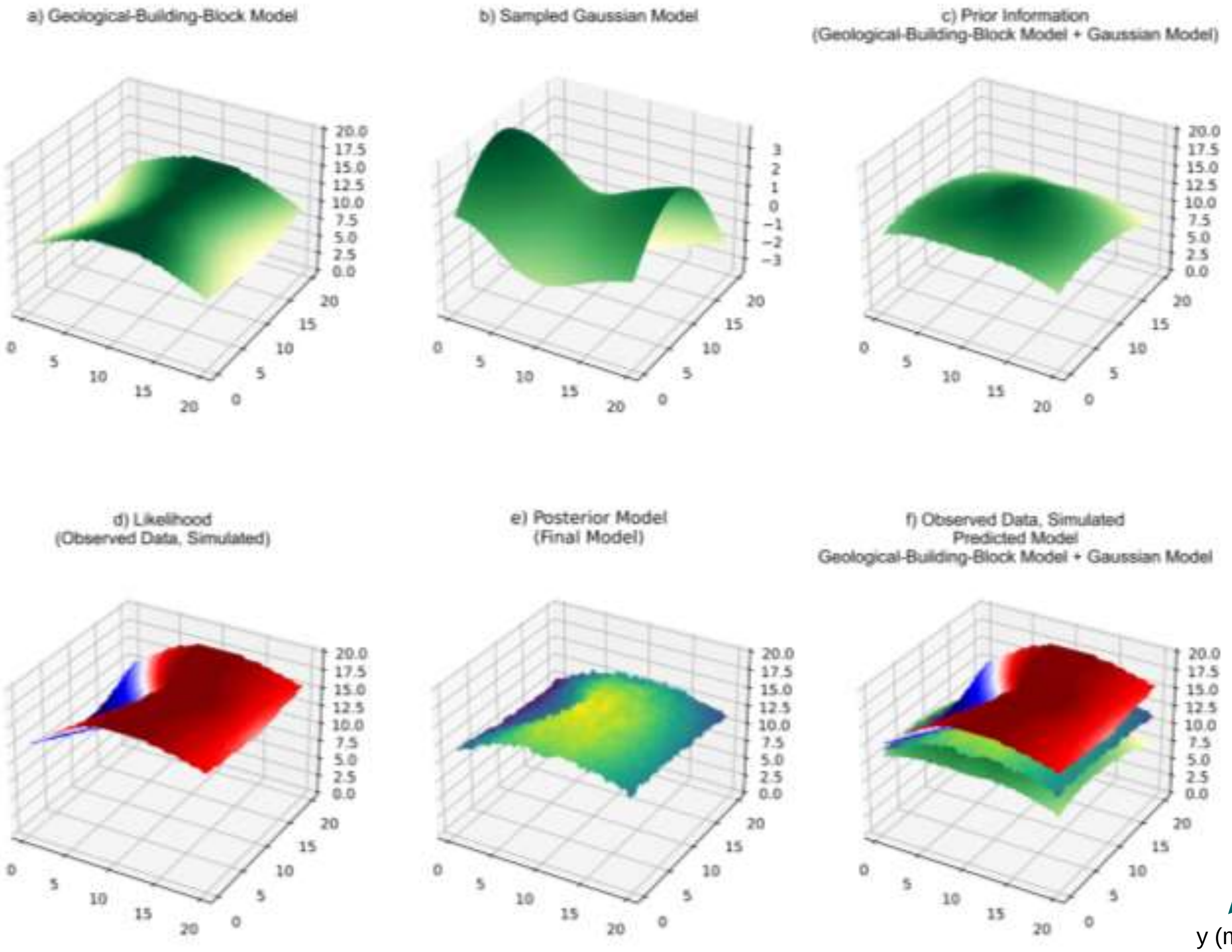
b) **Create Gaussian surface within the uncertain volume**

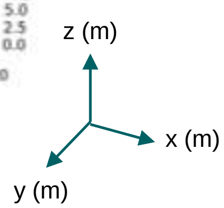
c) **Add previous surfaces to get the mean of the prior model**

d) **Incorporate observations as likelihood**

e) **Predict adaptation, posterior model**

f) ***Prior, Likelihood and Posterior***





Python Programming language GemPy PyMC3 NumPy matplotlib

Discussion

Discussion

- The reduction of the spatial uncertainty in the spatial definition of the geometrical structures is based on model adaptation to complementary information.

- The approach sets the base for further development on quantitative information and quantification.

- The likelihood function should be given by different types of observations.

- Variances are expected to address the uncertainty of the input data; simultaneously, the results obtained so far need to be smoothed to represent a realistic model.

Next Steps

Next Steps

- Review of the influence of the variances for the prior and likelihood.
- Application on real data.
- Addition of other means of information (e.g., gravity, magnetic and/or resistivity).
- Extend the review of methods to quantify uncertainties.

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Languages, packages and libraries:

- GemPy: https://gempy.org/, https://docs.gempy.org
- Matplotlib: https://matplotlib.org/
- NumPy: https://numpy.org/)
- PyMC3: https://www.pymc.io/projects/docs/en/v3/index.html
- Python: https://www.python.org/

Thank you for your attention

Questions?