GeoBlocks: Comparison between different kernel based methods in modeling host rock geometry for nuclear waste disposal

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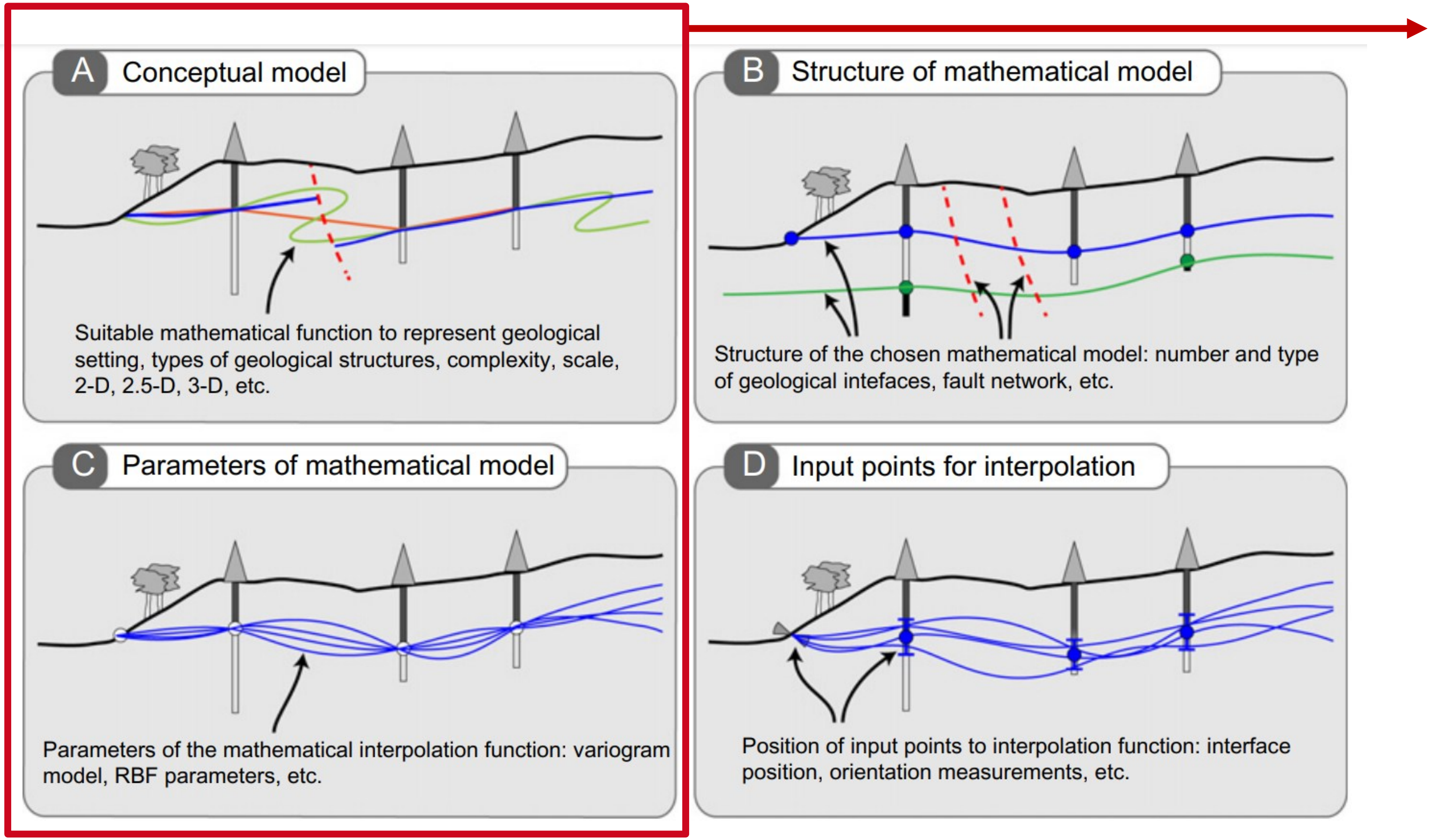
Background and Objective

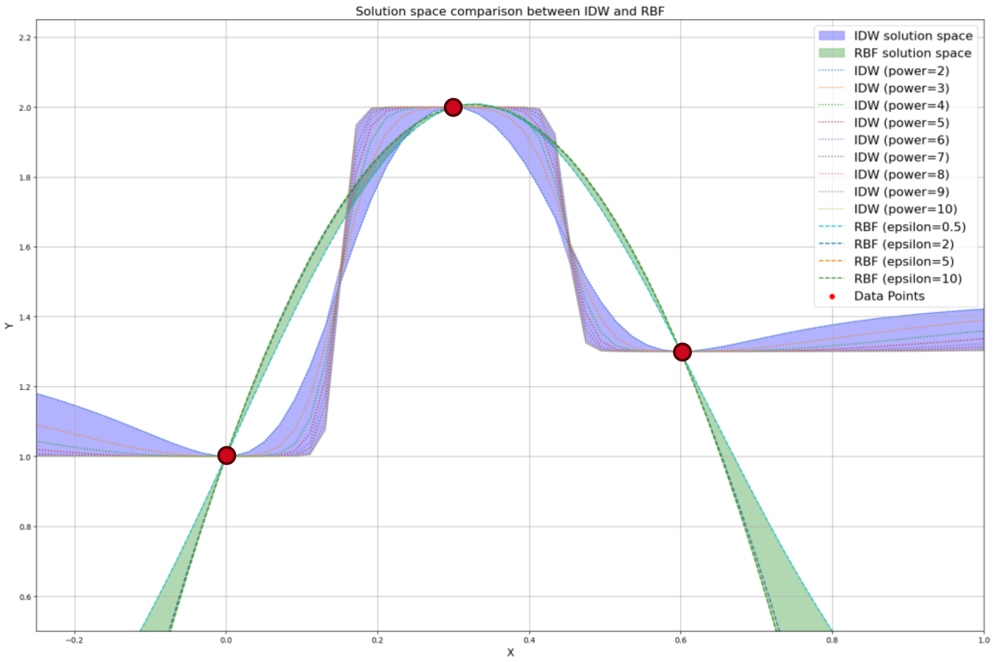


- Different methods and their parameters will generate different models.
- There is no single best modeling method for all situations; instead, there is an appropriate method for each individual model.
- The key to finding the proper method lies in the model comparison process.

Sources and types of uncertainty related to different modeling steps (Wellmann & Caumon, 2018).

Background and Objective

- Different interpolation methods have different **solution space**, which may fit **different host rock structures**.



Example: interpolation between three data points using IDW and RBF in 1D

IDW (Inverse Distance Weighting)

$$Z(x) = \frac{\sum_{i=1}^{N} \frac{Z_i}{d(x,x_i)^p}}{\sum_{i=1}^{N} \frac{1}{d(x,x_i)^p}}$$

Power: 2 to 10

RBF (Radial Basis Function)

$$Z(x) = \sum_{i=1}^{N} \lambda_i \, \phi(||x - x_i||)$$

Bandwidth: 0.5 to 10

Kernel function (gaussian)

$$\phi(r) = e^{-(\epsilon r)^2}$$

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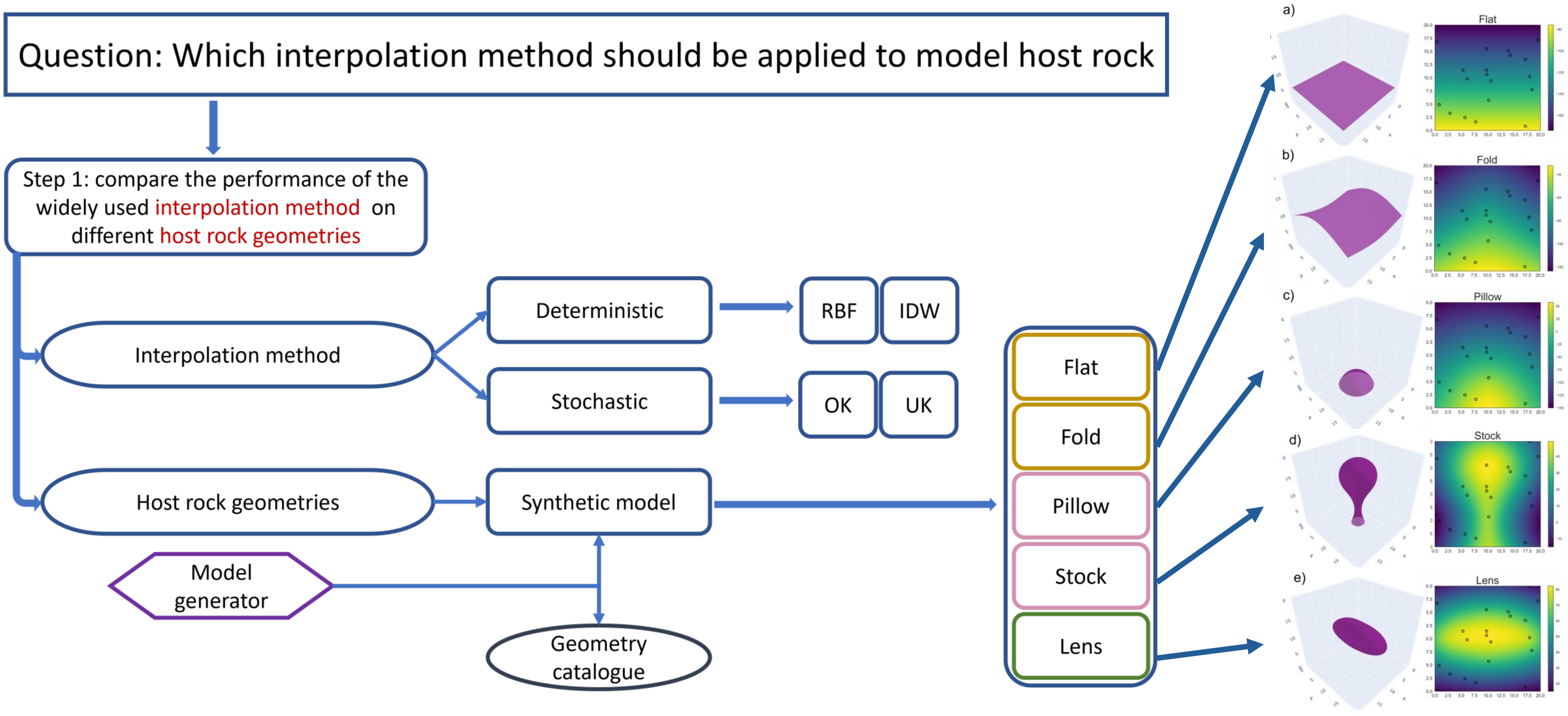
Previous Work



Previous Work

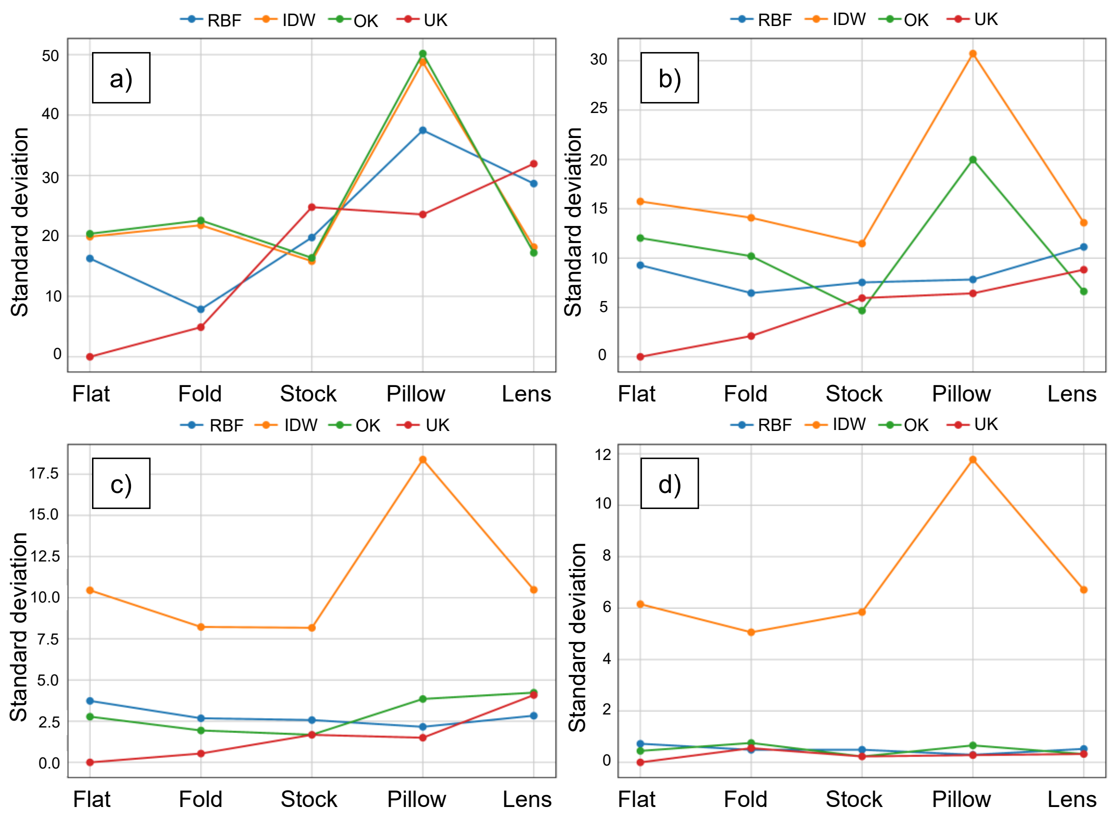


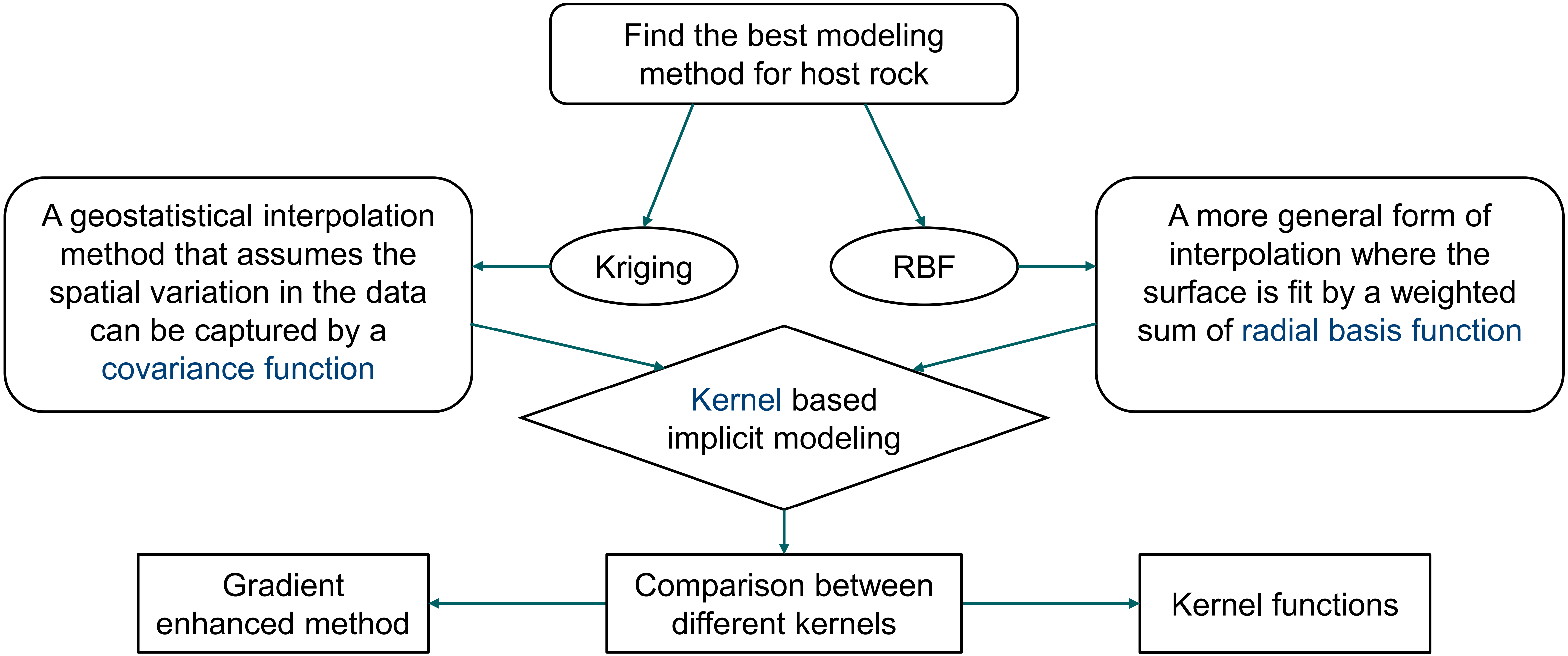
Figure: Standard deviation of cross-validation result for different density of sample points. (a)5 points (b) 20 points (c) 50 points (d) 200 points

- **Cross-validation(leave-one-out)**

One input data point is removed at a time, and the interpolation is performed for the location of the removed point using the remaining samples. The residual between the actual value of the removed data point and its estimate is then calculated. This process is repeated iteratively until every sample has been interpolated.

Kriging and RBF > IDW

Kernel Based Implicit Modeling

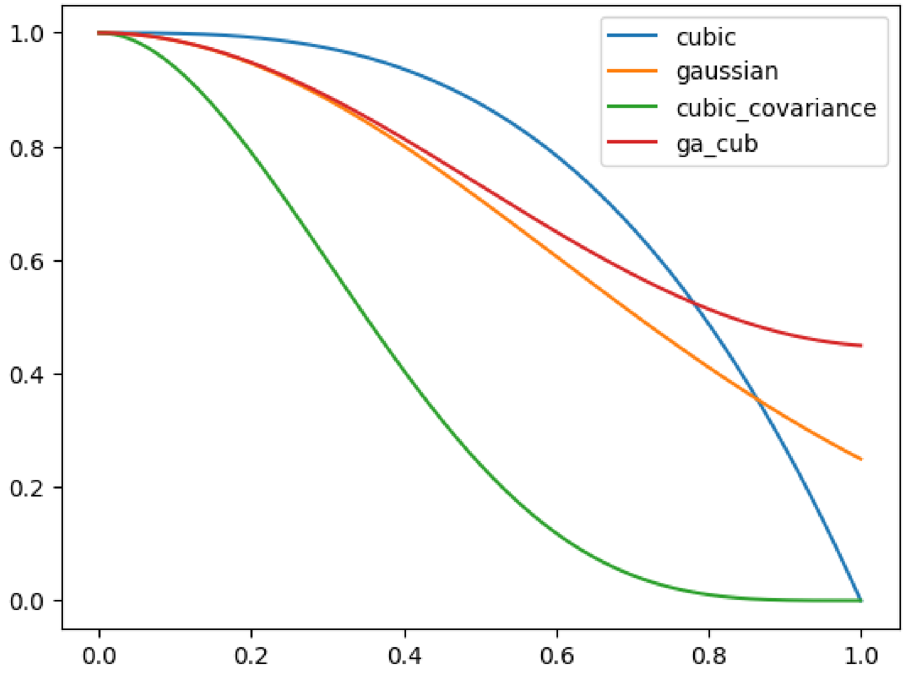


Different Kernels

$$Z(x) = \sum_{i=1}^{N} \lambda_i \, \phi(||x - x_i||)$$

$$\phi(d) =$$

Cubic	$1 - d^3$
Gaussian	$\exp\left(-\frac{d^2}{2\varepsilon^2}\right)$
Cubic covariance	$1 - 7\left(\frac{d}{r}\right)^2 + \frac{35}{4}\left(\frac{d}{r}\right)^3 - \frac{7}{2}\left(\frac{d}{r}\right)^5 + \frac{3}{4}\left(\frac{d}{r}\right)^7$
Gaussian and cubic hybrid	$\exp\left(-\frac{d^2}{2\varepsilon^2}\right) + n \cdot d^3$

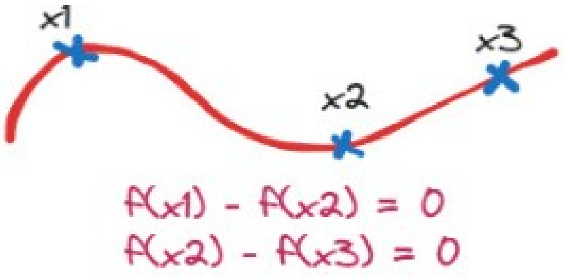


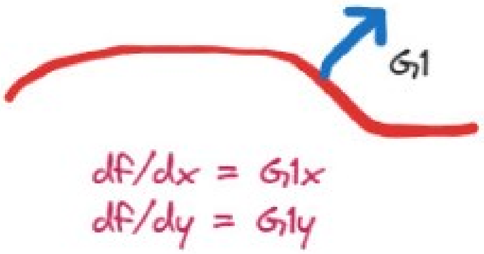
Gradient Enhanced Method

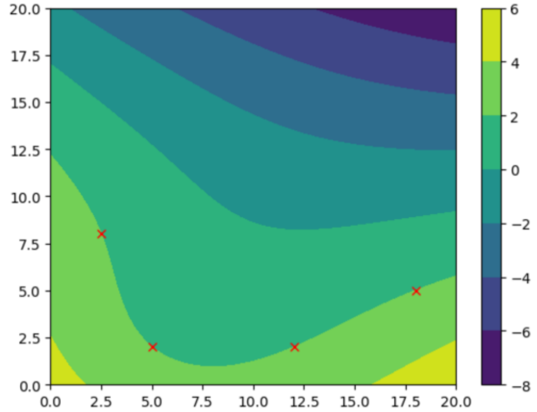
- General interpolation method only use coordinate and its value as input data.
- But in geological modeling, we also use orientations as additional input data.

Foliation field method (also the basic logarithm in GemPy)
(Lajaunie, C., Courrioux, G. & Manuel, L. Foliation fields and 3D cartography in geology: Principles of a method based on potential interpolation. Math Geol 29, 571–584 (1997). https://doi.org/10.1007/BF02775087)

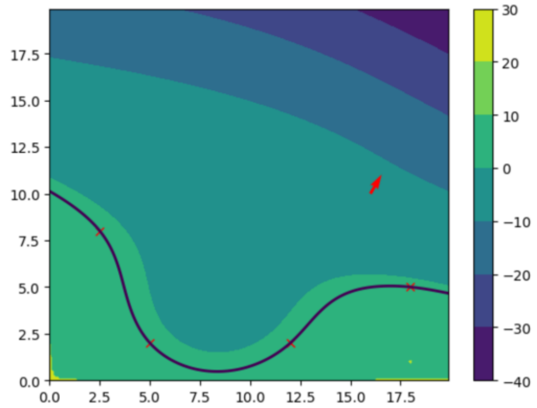
Follow two constraints:
- Surface points: the points in the same layer must have 0 increments.
- Orientation points: the gradients of data must equal to the input orientation.







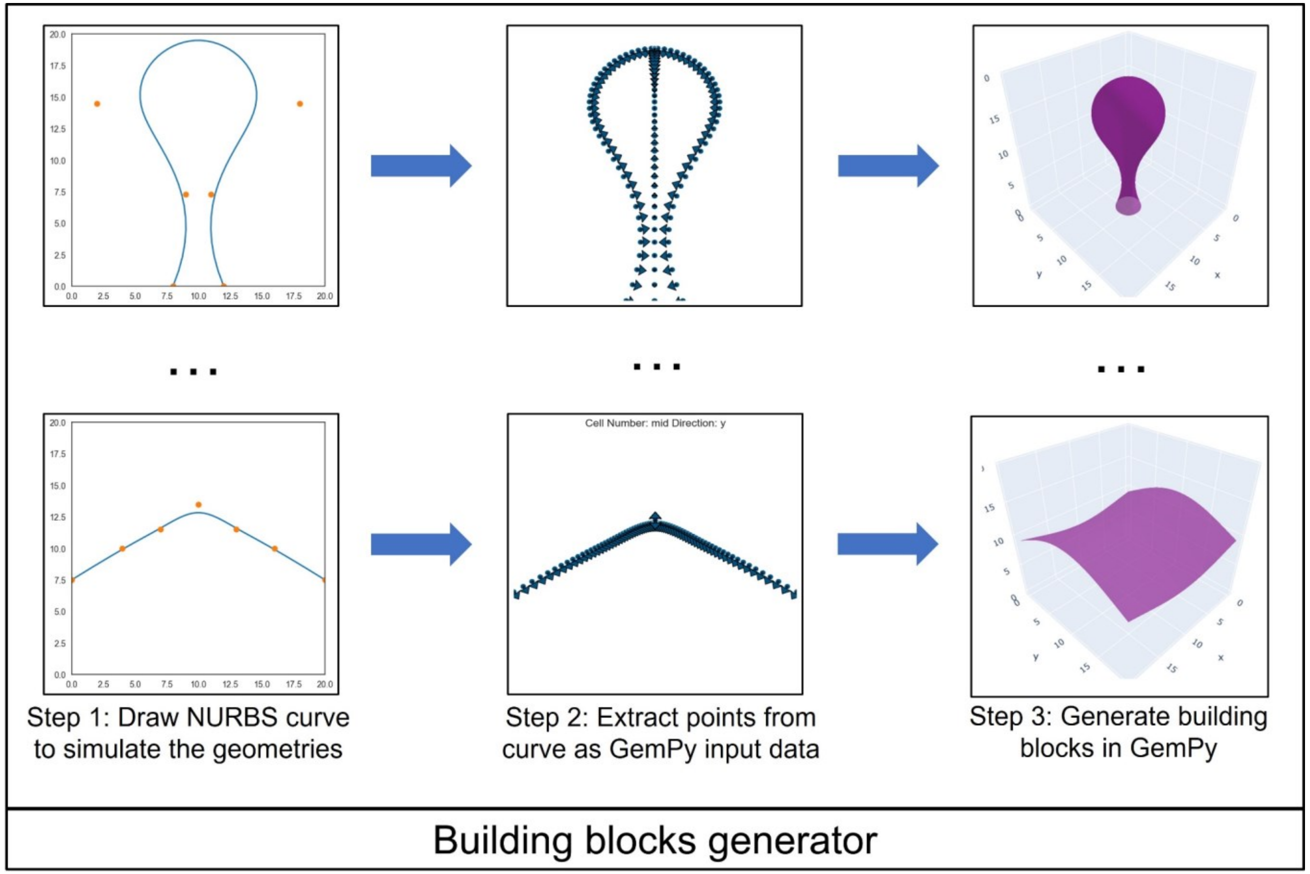
RBF without gradient



RBF with gradient

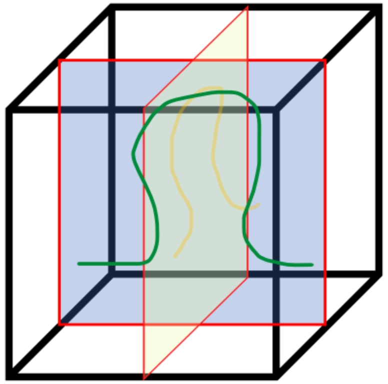
Model Generation

GemPy model generator V1.0



Fundamentals:

- Use NURBS (a basic curve formed by control point) to simulate the drawing of geometries
- The geometries are two cross-sections which are perpendicular to each other



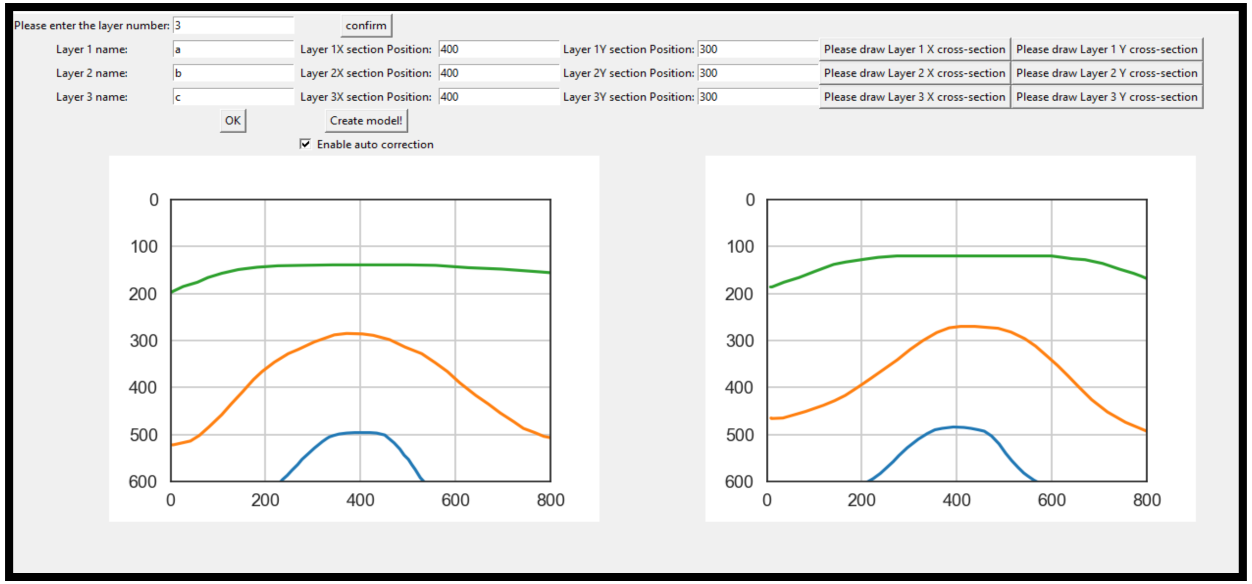
Advantages:

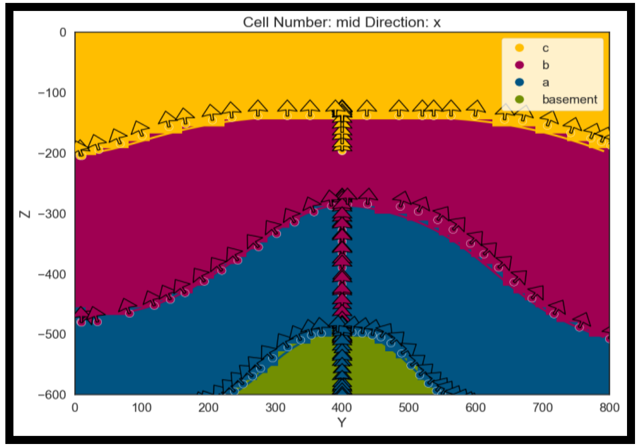
- Only 7 points to manipulate
- Easy to build a regular geometry

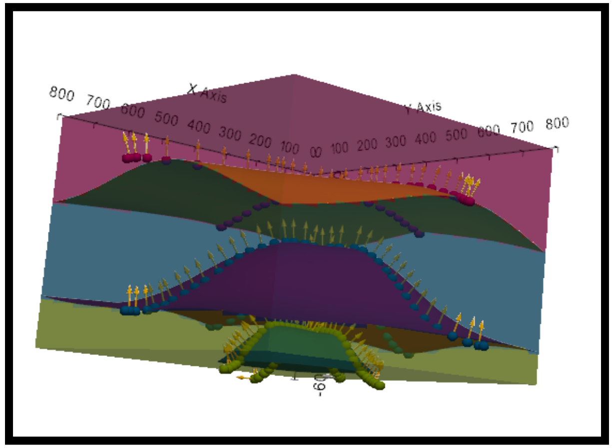
Disadvantages:

- Only allow one layer and two cross-sections
- Cannot build complicated geometry

Model Generation







GemPy model generator V2.0

https://youtu.be/U6YuCHWeSCs

Fundamentals:

- Use drawing curve to form the geometry
- Use GUI as import

Advantages:

- Allow multiple layers and cross-sections
- Easy to build complicated geometry
- A background image can be used as reference for drawing

Disadvantages:

- Hard to control the regular shape

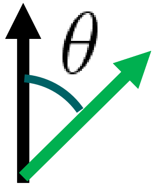
Model Comparison Method

There are a lot method can be applied to explicit and/or implicit volumetric structural models:

- Computing metrics for each model and the difference between these metrics
- (e.g., connectivity metrics, Thiele et al, 2016)
- Computing distance between models (e.g., The Haudorff distance between layers, Suzuki et al, 2008)
- Characterizing an ensemble of models (e.g., with information entropy from rock units indicators, Wellmann & Regenauer-Lieb, 2012)

Here we focus on subsets of implicit models described by one continuous scalar field

(Guillaume Caumon. On some comparison metrics between 3D implicit structural models. IAMG 21st annual conference, 2022, Nancy, France. ⟨hal-04165710⟩)

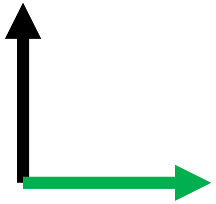


$$d^{\nabla}_{AB}(\mathbf{x}) = 1 - \frac{\nabla f_A \cdot \nabla f_B}{\|\nabla f_A\| \|\nabla f_B\|}$$

$$\frac{\nabla f_A \cdot \nabla f_B}{\|\nabla f_A\| \|\nabla f_B\|} = \cos(\theta)$$

$\theta = 0$

$d^{\nabla}_{AB}(\mathbf{x}) = 0$



$\theta = 90$

$d^{\nabla}_{AB}(\mathbf{x}) = 1$

$\theta = 180$

$d^{\nabla}_{AB}(\mathbf{x}) = 2$

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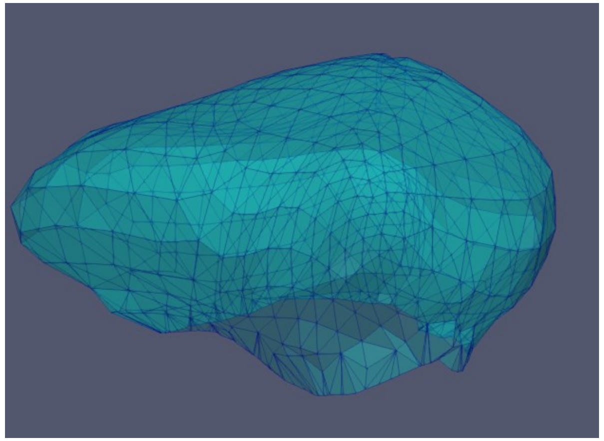
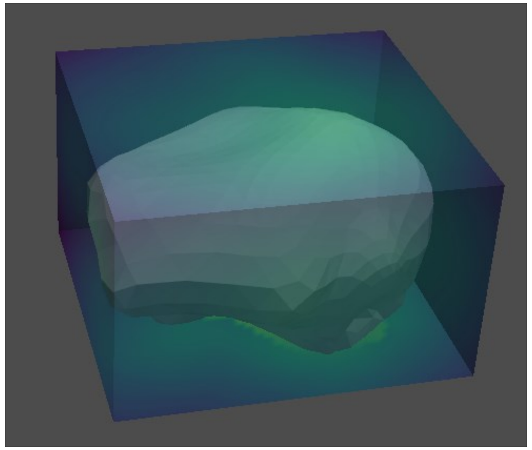
Salt Model

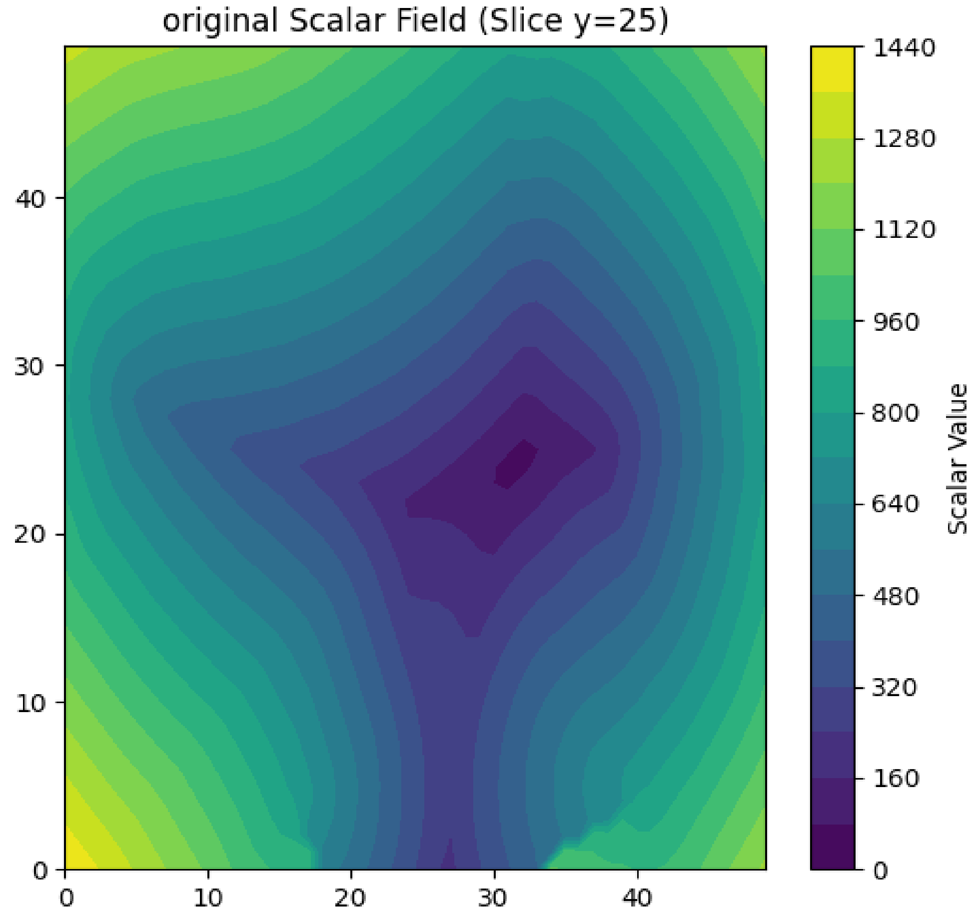


Model from TUNB



Create scalar field using pyvista compute_implicit_distance

(J. A. Baerentzen and H. Aanaes, "Signed distance computation using the ***angle weighted pseudonormal****," in IEEE Transactions on Visualization and Computer Graphics, vol. 11, no. 3, pp. 243-253, May-June 2005, doi: 10.1109/TVCG.2005.49.)*



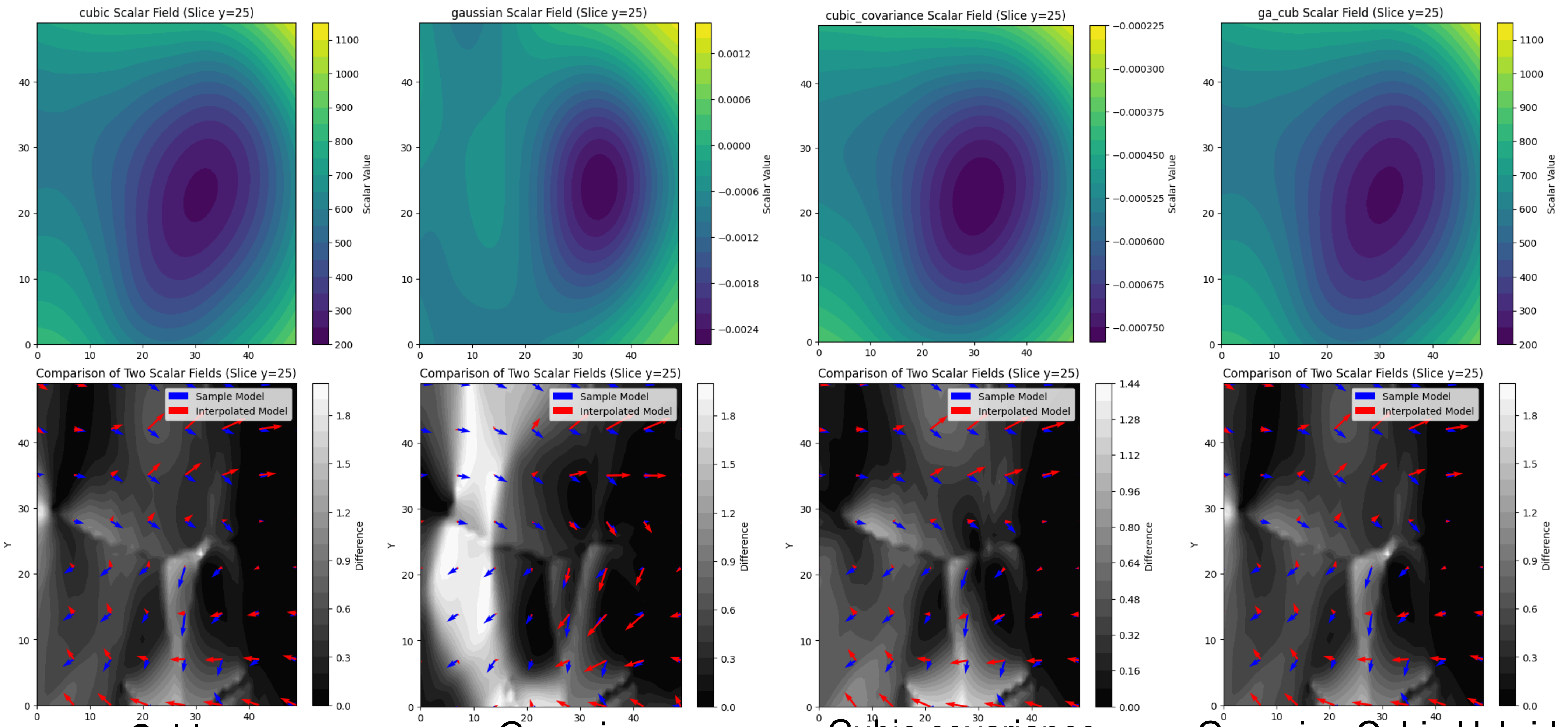
The cross-section in the mid-y axis

Interpolated Scalar Field and Differences

Samples: 50 points
5 gradients

Interpolated Scalar field Slice in mid-y axis

Difference Plot

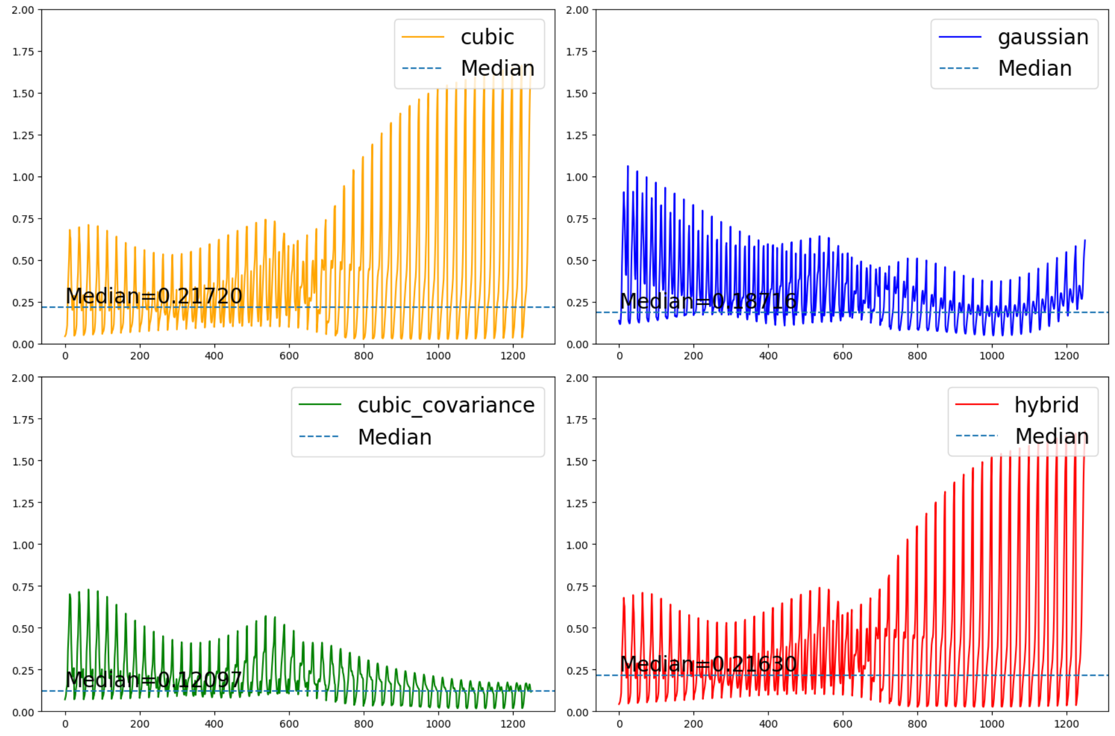


Kernels	Cubic	Gaussian	Cubic covariance	Gaussian Cubic Hybrid
Median	0.12855	0.24375	0.11192	0.12854

Difference Analysis

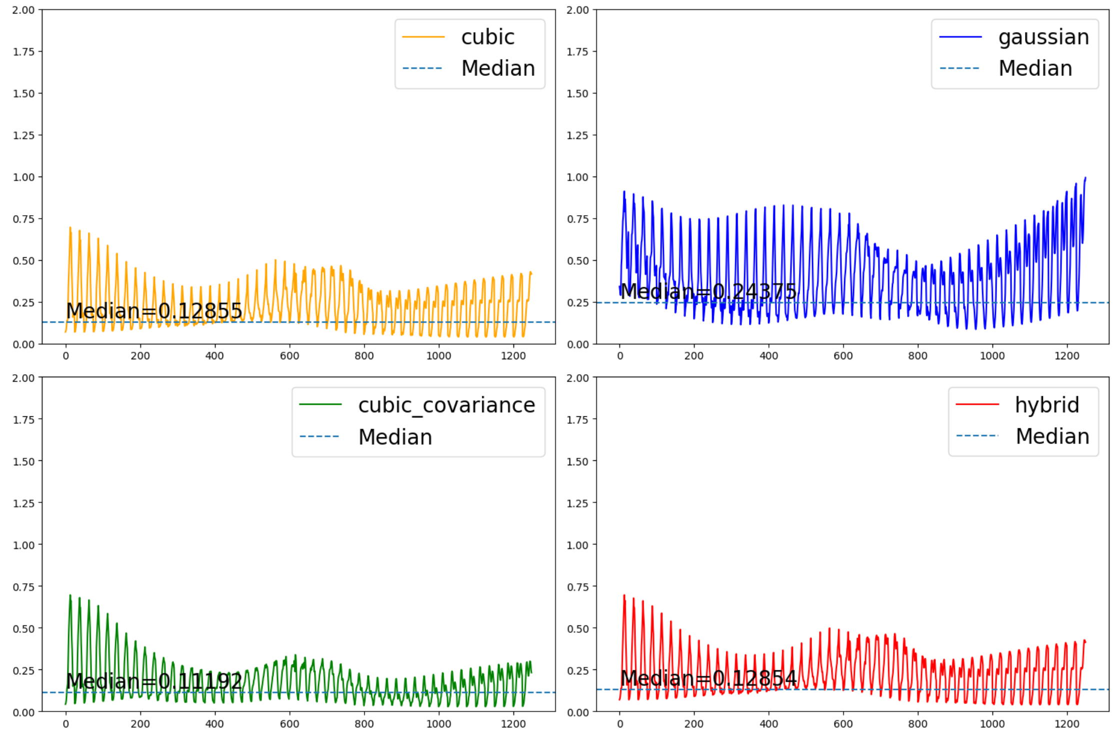
difference

10 points 1 orientations



grid points in the scalar field

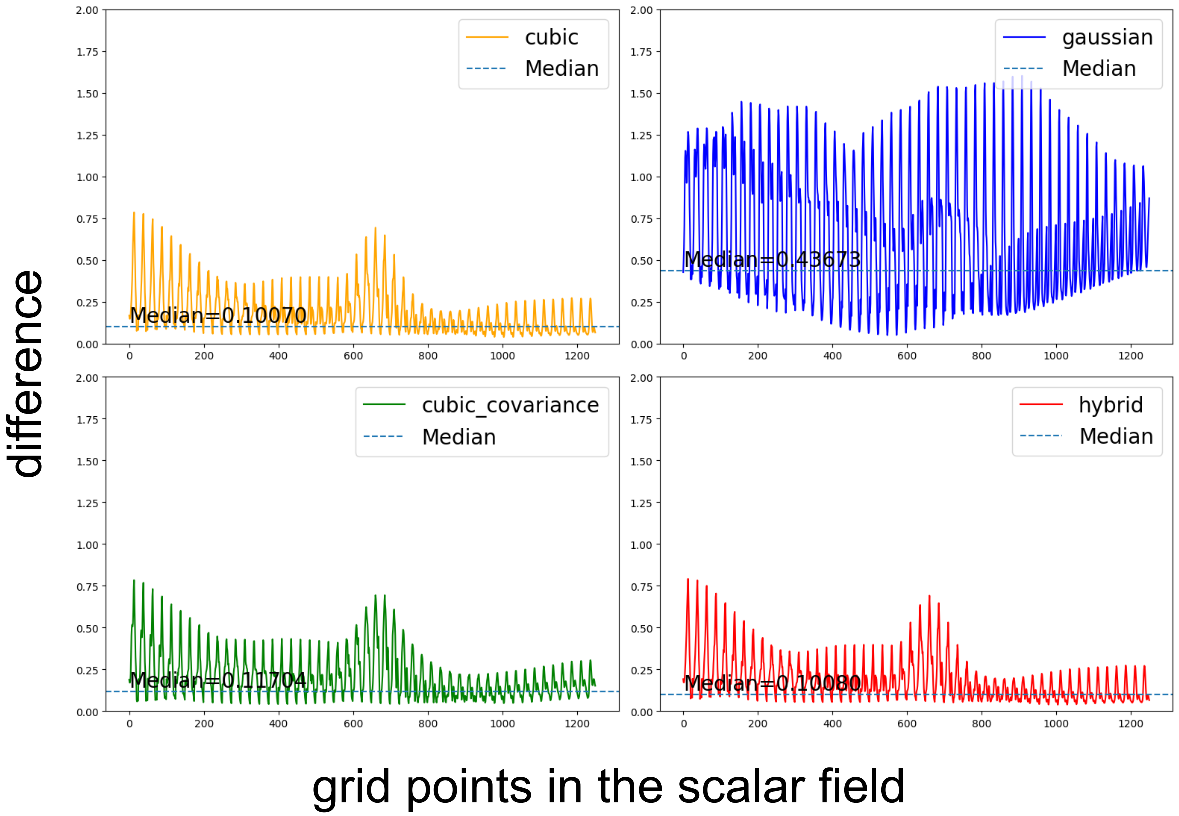
50 points 5 orientations



grid points in the scalar field

Difference Analysis

200 points 20 orientations



Future Work

- **Optimization of Hybrid Kernel Weights**: The hybrid kernel method shows significant potential for enhanced performance with appropriately assigned weights. Future research should focus on developing automated techniques for selecting optimal hybrid weights.

$$\exp\left(-\frac{d^2}{2\varepsilon^2}\right) + n \cdot d^3$$

- **Comprehensive Geometry Testing**: Expanding the range of geometries tested is crucial for identifying the most effective modeling methods for different shapes and structures.

- **Parameter Tuning for Various Kernels**: Further investigations are necessary to fine-tune the parameters for different kernels. This involves extensive testing to determine the optimal settings for various types of kernels, ensuring that they perform effectively under diverse conditions.

$$\exp\left(-\frac{d^2}{2\varepsilon^2}\right)$$

$$1 - 7\left(\frac{d}{r}\right)^2 + \frac{35}{4}\left(\frac{d}{r}\right)^3 - \frac{7}{2}\left(\frac{d}{r}\right)^5 + \frac{3}{4}\left(\frac{d}{r}\right)^7$$