

Materials and Methods: A QGIS Plugin for Three-Dimensional Implicit Geological Modelling and Uncertainty Estimation

1 Materials and Methods

1.1 Software Architecture and Input Data

The tool is implemented as a plugin for QGIS (≥ 3.40) written in Python 3, and couples the geographic-data handling of QGIS with the open-source implicit geomodelling engine GemPy [1]. It is designed to let a user move directly from georeferenced field data held in a QGIS project to a three-dimensional structural model and its associated uncertainty, without leaving the GIS environment.

Three input layers are required and are read directly from the active QGIS project: (i) a *surface-point* layer, in which each vertex carries planar coordinates (X, Y) , an elevation Z and a categorical *formation* attribute; (ii) an *orientation* layer, in which each measurement carries a location, a dip and a dip-azimuth (or, equivalently, the components of the unit pole vector) and a polarity; and (iii) a digital terrain model (DTM) supplied as a raster. An optional polygon layer may be used to define an area of interest (AOI) that clips the modelling domain. Vector layers in any QGIS-supported format are internally converted to a tabular representation, and all layers are required to share a common coordinate reference system (CRS) so that the geological observations and the topography are co-registered.

1.2 Implicit Structural Modelling

The structural model is computed with GemPy, which reconstructs geological interfaces as iso-surfaces of a continuous scalar (potential) field interpolated from the surface points and orientation data by a co-kriging scheme [1]. Formations are organised into ordered *structural groups* whose stratigraphic and tectonic relationships are specified by the user as **ERODE**, **ONLAP**, **FAULT** or **BASEMENT** relations; faults are detected automatically from formation names and may offset the remaining series according to configurable fault relations. The modelling domain is discretised on a regular grid whose horizontal extent is derived from the DTM (or the AOI) and whose vertical extent spans from a user-defined basal depth to the maximum terrain elevation. The DTM is incorporated as the upper boundary of the model, so that geological surfaces are truncated at the topography. After interpolation, the explicit triangulated surfaces of each interface are extracted from the scalar field and rendered interactively in an embedded PyVista [3] viewer.

1.3 Mesh Generation and Export

Each geological interface and the topographic surface can be exported as a watertight triangular mesh in STL format for downstream use (e.g., 3D printing or numerical simulation). The topographic solid is generated by Delaunay triangulation of the DTM nodes and vertical extrusion to the model base, while the structural surfaces are taken from the interpolated iso-surfaces. Prior to export, all meshes are passed through a cleaning and repair stage—coincident-vertex merging, consistent normal orientation, and topological repair with the MeshFix algorithm [4]—and the

terrain is optionally smoothed (Gaussian filtering of the elevation field only, preserving the planimetric footprint and hence the CRS). This step removes non-manifold edges, self-intersections and folded faces that would otherwise compromise meshing downstream.

1.4 Uncertainty Estimation by Monte Carlo Perturbation

Because orientation measurements are the input most affected by observational error, the tool quantifies structural uncertainty through a Monte Carlo ensemble in which the orientation data are perturbed and the model is recomputed [2]. For each of N realisations, every orientation is independently perturbed by adding Gaussian noise to its dip and dip-azimuth,

$$\delta_k \sim \mathcal{N}(\delta_0, \sigma_\delta^2), \quad \alpha_k \sim \mathcal{N}(\alpha_0, \sigma_\alpha^2), \quad (1)$$

where δ_0 and α_0 are the measured dip and azimuth, and σ_δ and σ_α are user-defined standard deviations (default 5° and 10° , respectively); dips are clipped to the physically admissible range and azimuths are wrapped modulo 360° . The full model is rebuilt and recomputed for each realisation, keeping the geometry, grid and structural configuration fixed, so that the only source of variability is the orientation noise.

Each realisation k yields a discrete lithology label $l_i^{(k)}$ for every grid cell i . Aggregating across the N realisations gives, for every cell, the relative frequency of each lithology l ,

$$p_i(l) = \frac{1}{N} \sum_{k=1}^N \mathbb{1}[l_i^{(k)} = l]. \quad (2)$$

From this distribution the tool derives, per cell: the *modal lithology* $\hat{l}_i = \arg \max_l p_i(l)$; the *modal probability*

$$P_i = \max_l p_i(l), \quad (3)$$

a confidence measure that approaches 1 where realisations agree and decreases where they diverge; and the *information (Shannon) entropy*

$$H_i = - \sum_l p_i(l) \ln p_i(l), \quad (4)$$

which is zero where a single lithology is always predicted and maximal where several lithologies are equally likely [2]. The resulting probability, entropy and modal-lithology volumes are written to disk as gridded arrays (together with the model extent) and can be explored as interactive cross-sections. Summary statistics—the mean modal probability, the mean entropy, and the fraction of cells whose modal probability falls below a confidence threshold (0.8)—are reported to characterise the overall reliability of the model.

References

- [1] de la Varga, M.; Schaaf, A.; Wellmann, F. GemPy 1.0: open-source stochastic geological modeling and inversion. *Geosci. Model Dev.* **2019**, *12*, 1–32.
- [2] Wellmann, J.F.; Regenauer-Lieb, K. Uncertainties have a meaning: Information entropy as a quality measure for 3-D geological models. *Tectonophysics* **2012**, *526–529*, 207–216.
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- [4] Attene, M. A lightweight approach to repairing digitized polygon meshes. *Vis. Comput.* **2010**, *26*, 1393–1406.