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The Piecewise Structural Complex: topology-constrained geological unit attribution using the Structural Topology Model in PZero 2.0

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Abstract. Geological modelling requires preserving not only the geometry of geological objects, but also their topological relationships and geological interpretation. In this work, we extend the implementation of the Structural Topology Model (STM) in PZero, an open-source geological modelling platform, by adding automatic topology-constrained Structural Level (SL) calculation and introducing the Piecewise Structural Complex (PSC), a topology-driven procedure for geological partitioning and unit attribution in two and three dimensions. In the STM graph, the set of geological boundary identities connected to each unit defines its global topological signature. The PSC compares these graph-derived signatures with the sets of boundary identities delimiting locally reconstructed closed regions. In 2D, PSC identifies closed areas delimited by geological boundary traces in cross-sections, whereas in 3D it identifies connected volumetric regions within a preliminary tetrahedral mesh. Both procedures use the same signature-matching logic: exact matches require identical boundary sets, whereas partial matches tolerate a user-defined number of missing expected boundaries but no unexpected observed boundaries. After PSCs have been generated and checked in 2D, seed points assigned in cross-sections allow geological unit assignments to be transferred to the 3D PSCs. Topographic information can additionally distinguish preserved subsurface from reconstructed eroded occurrences.

The implementation is tested through three synthetic 2D examples, one synthetic 3D model, and two simplified real 3D case studies. These tests demonstrate that the combined STM–PSC workflows support topology-constrained SL calculation and accommodate incomplete local signatures, repeated units, finite structural discontinuities, and topographic subdivision while explicitly retaining ambiguous outcomes where automatic topological analysis cannot establish a unique geological attribution. The proposed approach therefore automates geological unit attribution where topological constraints are sufficient, while identifying cases that require expert interpretation.

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1 Introduction

3D geological modelling has experienced significant growth particularly over the past two decades, becoming an increasingly widespread tool in several fields of geosciences, ranging from structural geology to civil engineering, as well as mining, subsurface storage, and the energy sector (Mallet, 2002; Vollgger et al., 2015; Xiong et al., 2018). However, this development has not been uniformed across application fields or over time. Early developments were largely driven by capital-intensive sectors, particularly hydrocarbon exploration and mining, where the economic value of subsurface targets justified substantial investments in data acquisition, computing resources, and specialised modelling software (Power et al., 2001; Sides, 1997; Hartman and Mutmansky, 2002; Jahn et al., 2008).

The subsequent diffusion of 3D geological modelling into other fields has been facilitated by increasingly accessible computing resources and by the emergence of several open-source 3D modelling software and libraries (de la Varga et al., 2019; Grose et al., 2021; Bistacchi et al., 2021; Malard et al., 2023; Monti et al., 2024; Kamath et al., 2026).

However, topological challenges are still encountered in polymetamorphic orogens, where unconformities, tectonic contacts, transported or duplicated units, and other structural complexities can complicate the definition of a reliable stratigraphic framework (Fettes et al., 2011; Arienti et al., 2024; Monti et al., 2024; Simonetti et al., 2024; Musso Piantelli et al., 2026). In these contexts, the topology of geological units and surfaces is coupled with an ontological issue (Monti et al., 2026), since conventional stratigraphic classifications may be insufficient to consistently define the geological units and boundaries to be represented.

Although these challenges can be particularly restrictive in implicit modelling workflows, where geological interpolation often relies on predefined stratigraphic or structural ordering (Mallet, 2002; Tertois, 2007; Grose et al., 2021; Monti et al., 2026), they are not inherent to a specific modelling approach and may also affect explicit workflows, where the absence of formalized topological and ontological constraints can result in interpretative or operational inconsistencies.

As geological models become more complex, consistency must be maintained not only in the geometry of individual surfaces but also in the geological meaning and mutual relationships of the regions they delimit. This becomes particularly important because geological interpretations are commonly represented at different stages of a modelling workflow: as units and boundaries in a geological legend, as lines and polygons in cross-sections, as surfaces and volumes in three dimensions, and, where numerical applications are involved, as material regions and boundary sets in volumetric meshes. These representations describe the same geological interpretation, but they are not geometrically equivalent and therefore require an explicit mechanism to preserve their topological and semantic correspondence.

A watertight partition ensures that the model domain is unambiguously subdivided into regions, which is essential for visualisation, model interrogation, and subsequent numerical applications (Mallet, 2002; Caumon et al., 2004, 2009; Pellerin et al., 2017). The construction and management of such geometrically and topologically consistent partitions can be supported by dedicated tools, including MeshIt and the related PyMeshIt workflow (Cacace and Blöcher, 2015; Hussain et al., 2026), as well as libraries for representing and manipulating geological model topology, such as RINGMesh (Pellerin et al., 2017) and

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OpenGeode (Bonneau et al., 2024). However, the resulting regions still need to be associated with the geological units they represent. In complex settings, this association cannot always be inferred from stratigraphic order or spatial position alone, because the same unit may be repeated, truncated, displaced, or exposed through only part of its bounding relationships. A formal definition of geological topology is therefore required not only during model construction, but also to propagate geological meaning between different geometrical representations of the model (Hussain et al., 2026; Monti et al., 2026).

Formal representations of geological relationships have been explored through knowledge-based chrono-spatial rules (Perrin et al., 2005), as well as approaches to extract and analyse spatial and temporal topology (Thiele et al., 2016a, b; Jessell et al., 2021; Grose et al., 2021), constrain stochastic geological models using topological information (Schaaf et al., 2021), and assess geological model consistency using spatial, temporal, and polarity constraints (Parquer et al., 2025). These contributions provide important foundations for the formalisation of geological knowledge and relationships, although the correspondence between geological units defined in an interpretative framework and geometrically reconstructed regions remains a yet open modelling problem.

To formalise geological knowledge independently of geometric reconstruction, Monti et al. (2026) proposed the Structural Topology Model (STM), a topological and ontological framework aimed at formalizing the relationships between structural level (SL), geological units, and boundaries across 2D and 3D geological representations. This framework provides an advantage in the construction of consistent geological 2D and 3D modelling legends, even for highly complex settings. However, an additional procedure is needed to associate the geometrical regions resulting from model partitioning with the units and relationships defined in the STM legend.

In this work, we introduce the Piecewise Structural Complex (PSC), a topology-driven procedure to associate geometrically defined regions with the geological units represented in an STM legend. The method compares the topological signatures derived from the STM graph with those obtained from closed polygons in geological cross-sections (2D) or connected volumetric regions in tetrahedral meshes (3D). The same matching principles apply to both representations, supporting exact and partial matches, structural repetitions, and ambiguous or unresolved assignments without imposing a unique interpretation where topological information is insufficient. We present the underlying procedure and its implementation in PZero, an open-source Python-based geological modelling platform (https://github.com/gecos-lab/PZero; Bistacchi et al., 2021), including the graphical tools developed for constructing and managing STM graphs and applying PSC to 2D and 3D geological models.

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2 The Structural Topology Model

The Structural Topology Model (STM; Monti et al., 2026), is a conceptual and topological framework for constructing geologically consistent legends by explicitly defining the relationships between geological units and boundaries. According to the classification of Guarino (1998), STM constitutes an application ontology, formalising geological entities and their relationships independently of their geometrical representation.

STM provides the geological reference used by the Piecewise Structural Complex (PSC) to associate geometrically defined regions in 2D cross-sections and 3D models with the units of the underlying geological legend. The following section only recalls the elements of the framework required for understanding these procedures, as this work is considered as a continuation of the previous publication (Monti et al., 2026).

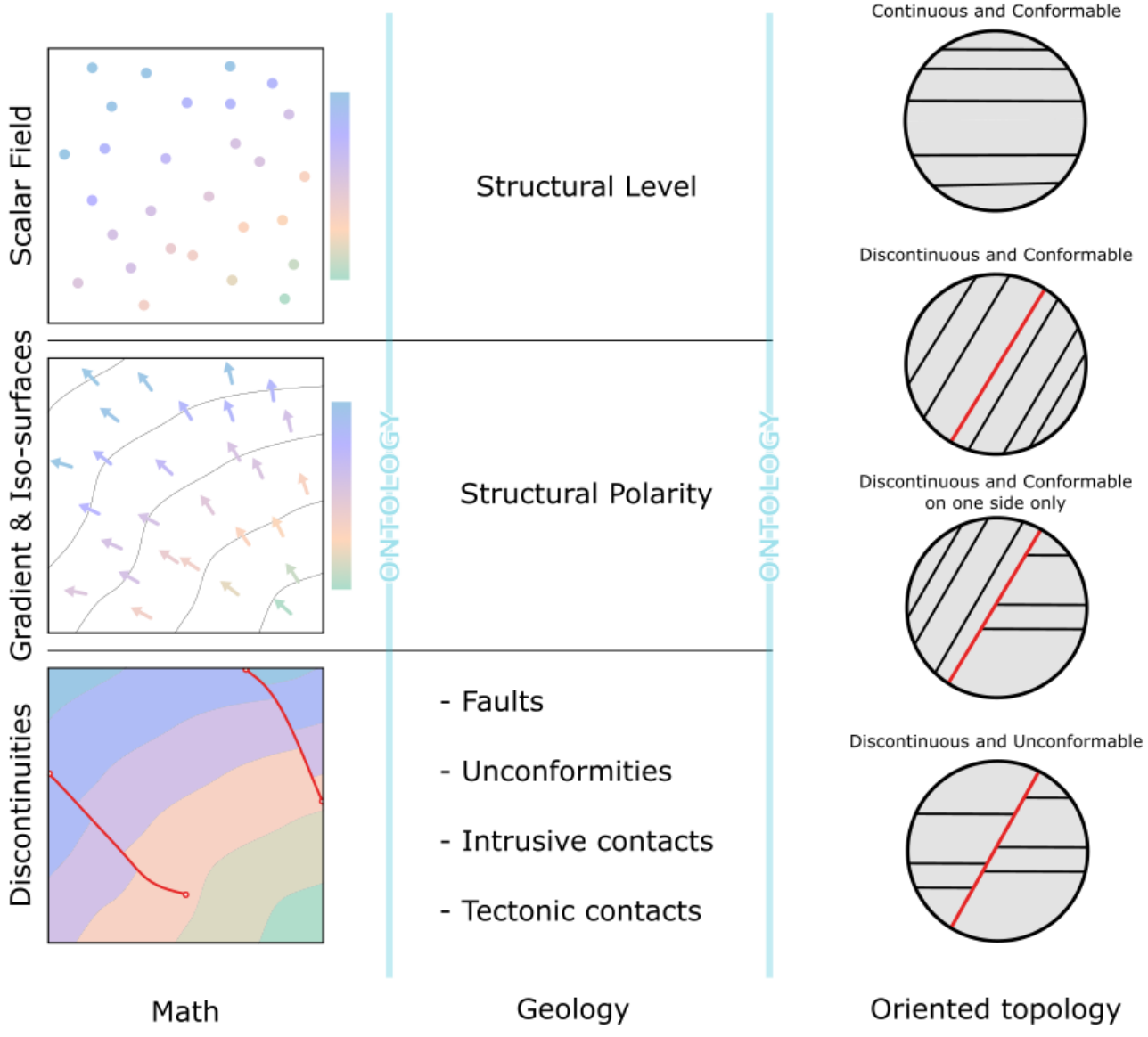
2.1 Structural Scalar Field

To consistently represent geological structures and stratigraphy in 3D, STM generalises the scalar-field approach of implicit geological modelling through the concept of a Structural Scalar Field. This provides a conceptual framework (Fig. 1) that can also be applied to 2D geological representations and explicit modelling workflows, without requiring the actual interpolation of the scalar field.

The field is described by Structural Level (SL), a scalar quantity whose values can be defined using absolute ages (geochronological and chronostratigraphic), relative temporal relationships (e.g., cross-cutting relationships), and structural criteria (e.g. structural position). The gradient of the SL field defines Structural Polarity (SP), a vector field normal to its isosurfaces, which may represent the younging direction in stratigraphic contexts or the direction normal to foliation in structurally complex units.

Geological discontinuities, such as faults and unconformities, may interrupt the continuity of SL. To describe their relationships with the surrounding units, Monti et al. (2026) introduced the concept of oriented topology, combining the continuity of the scalar field across a boundary with its conformability to the internal bedding or foliation of the adjacent units. With oriented topology, four classes of boundaries are defined: (1) continuous and conformable (absence of discontinuities), (2) discontinuous and conformable (e.g., depositional hiatus and thrusts), (3) discontinuous and conformable on one side only (e.g., unconformities and tectonic contacts), and (4) discontinuous and unconformable on both sides (e.g., faults).

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120 **Figure 1: Conceptual basis of the Structural Topology Model (STM), linking mathematical, geological, and oriented topological representations. Structural Levels (SLs) and the associated scalar-field representation constrain geological units and boundaries, while the four end-member boundary classes illustrate the possible combinations of continuity and conformability. Modified from Monti et al. (2026).**

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125

2.2 Units and Boundaries

In boundary representation (BREP) models, stratigraphic, intrusive, and tectonic boundaries, together with an external model boundary, partition the modelling domain into watertight volumes representing geological units (Braid, 1975; Mallet, 2002; Caumon et al., 2004). With STM, units are classified in tectonic units (TUs), stratigraphic units (SUs), and intrusive units
130 (IUs), according to their geological evolution and based on observable, interpretable, and mappable parameters at the scale of representation.

A particular subclass of TUs is represented by Structural Domains (SDs). These represent volumes characterised by distributed deformation or structural properties rather than strictly lithological boundaries.

Within STM, boundaries are not merely geometrical interfaces, but also represent geological entities with specific meanings
135 and relationships to the surrounding units. Changing the geological role of a boundary (without modifying its geometry) may therefore substantially alter the geological interpretation of the model.

Conformability is defined for each unit–boundary relationship, rather than as an intrinsic property of a boundary. The same surface may therefore be conformable with respect to one unit and unconformable with respect to another.

STM also accounts for hierarchical relationships among geological objects, which may vary with modelling scale and
140 resolution. Units and boundaries can therefore be organised at different hierarchical levels according to their topological relationships, allowing locally detailed subdivisions to be embedded within broader geological domains.

These relationships are represented in the STM graph, where geological units and boundaries constitute nodes connected by links expressing their conformable or unconformable relationships. The overall ontological architecture of STM, including the relationships among geological entities, oriented topology, and Structural Level, is summarised in Fig. 2. SL values provide
145 an ordering of geological entities, whereas the unit–boundary relationships define the topological information subsequently used by PSC to identify geological units within geometrically reconstructed regions.

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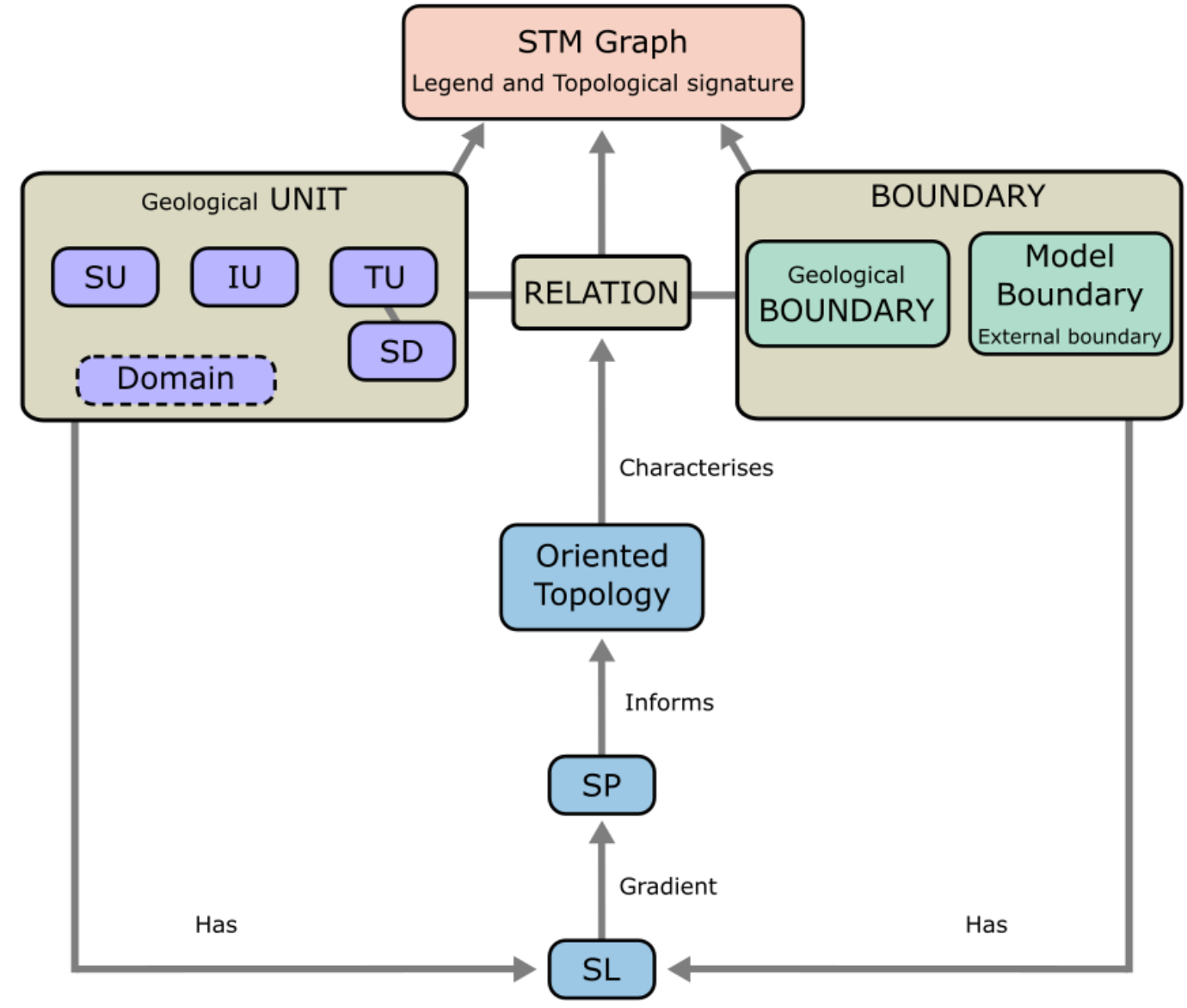


Figure 2: Conceptual architecture of the STM. Modified from Monti et al. (2026).

150

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3 Piecewise Structural Complex

The Piecewise Structural Complex (PSC) provides a topology-driven procedure to associate a geometrical partition of either a 2D cross-section or a 3D model with the geological units defined in the STM, through the comparison of their topological signatures. Although the construction of these regions differs between 2D and 3D, both workflows derive a local topological description of each region and compare it with the same STM information. The PSC therefore provides a common conceptual and computational link between the global geological interpretation encoded in the STM and its local geometrical expression. A single geological unit may correspond to multiple disconnected geometrical regions, for example as a result of tectonic repetition, while individual regions may expose only a subset of the boundaries associated with that unit in the global STM. Consequently, geological attribution cannot rely on a one-to-one correspondence between units and geometrical regions, but requires the comparison of their topological relationships.

3.1 STM graph and topological signatures

The relationships between geological units and boundaries defined in the STM can be formally represented as a bipartite graph (Borgatti and Everett, 1997; Latapy et al., 2008; Diestel, 2017):

$$G_{STM} = (U \cup B, E), \quad E \subseteq U \times B, \quad E = E_C \cup E_U, \tag{1}$$

where U is the set of geological units, B is the set of boundaries, and E contains the relationships connecting units and boundaries, based on oriented topology (conformable E_C or unconformable E_U). Each boundary node represents a conceptual boundary entity rather than an individual geometrical object. A single boundary may therefore be represented by multiple geometrical objects while retaining the same identity within the STM graph.

For a generic unit u, the sets of conformable B_C and unconformable B_U boundaries b connected to it are defined as:

$$B_C(u) = \{b \in B \mid (u, b) \in E_C\}, \qquad B_U(u) = \{b \in B \mid (u, b) \in E_U\}. \tag{2}$$

For the purposes of PSC matching, the global topological signature of a unit u is defined as the union of its conformable and unconformable boundaries:

$$S(u) = (B_C(u) \cup B_U(u)). \tag{3}$$

The global signature $S(u)$ therefore contains the identities of all geological boundaries associated with the unit, independently of their conformability. However, the distinction between $B_C(u)$ and $B_U(u)$ is preserved within the STM, as conformability provides an additional topological constraint used to validate repeated occurrences of the same geological unit (Sect. 3.4).

STM units may also be organised into optional domains representing an interpreted geological hierarchy (Sect. 2.2), representing higher-order geological groupings such as tectonic nappes, stratigraphic successions, or magmatic complexes. In the present formulation, domains do not constitute additional nodes of the STM graph, and unit–boundary relationships remain defined at the level of individual units. Consequently, topological signatures are associated with individual units rather than with their parent domains, preserving unit-level topology within the interpreted hierarchical organisation.

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3.2 Topology-constrained Structural Level assignment

SL is treated as a scalar coordinate expressing the relative structural position of geological objects by combining the ordering of boundaries, cross-cutting relationships, and geological interpretation. In the adopted convention, numerically lower values represent relatively higher structural positions. The relationships encoded in the STM graph, including boundary conformability and geological roles, can therefore be used to constrain the assignment of SL to geological units.

The use of relational constraints to establish admissible structural orderings is conceptually related to earlier approaches to geological event ordering (Burns, 1975) and the formalisation of temporal relationships (Allen, 1983; Michalak, 2005). However, unlike chronological ordering, SL does not necessarily represent geological time, but may instead express structurally meaningful relative positions (Monti et al., 2026).

Boundaries with an assigned SL define a sequence of structural intervals within which units can be positioned. If several units are constrained to the same interval, their relative ordering requires internal boundaries that can establish their relative separation. Where such a separator exists, alternative intermediate positions can be defined consistently with the possible ordering of the units. If no topological information is available to distinguish them, their relative positions remain unresolved.

The assignment of SL is primarily constrained by conformable boundaries with an assigned SL. When a unit is associated with two conformable boundaries with known SL, it can be positioned within the interval defined by their bounding SL values and assigned an intermediate value. When only one conformable boundary is available, the boundary acts as an anchor. Candidate positions are therefore retained on both sides of the boundary unless additional directional constraints apply. The unconformable boundaries associated with the unit provide additional topological support for one or the other candidate, without automatically excluding the alternative.

For SUs, top and base relationships also provide directional information: a top relationship supports a position toward higher numerical SL values, whereas a base relationship supports a position toward lower ones. An additional subset of conformable relationships E_L, identifies locked relationships:

$$E_L \subseteq E_C \tag{4}$$

When a SU is associated with a single conformable boundary with known SL, a locked relationship with a boundary classified as top or base provides a strong directional constraint, excluding positions on the opposite side. Conversely, non-locked top/base relationships provide only preferential directional information, while locked relationships involving other unit or boundary roles do not independently impose a directional constraint. Alternative solutions are retained when the topology does not allow an unambiguous choice.

The absence of a conformable boundary does not necessarily leave a unit unresolved. In this case, each connected boundary with a known SL can act as a possible anchor, and candidate positions can be defined in the adjacent structural intervals. Boundary incidence defines the set of admissible positions but does not, by itself, establish a preferred ordering among them. In particular, the occurrence of two connected boundaries at the limits of the same interval is not interpreted as evidence that

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the unit must occupy that interval. This prevents, for example, a unit connected to two faults from being automatically positioned between them solely because both faults occur among its associated boundaries.

Candidate positions are subsequently evaluated jointly for all units rather than independently. Admissible solutions correspond to globally compatible configurations of the STM. Configurations are rejected when they violate the imposed topological constraints, for example by placing multiple non-intrusive units within the same structural interval without a boundary capable of separating them, by placing multiple units on the same side of the same conformable boundary, by assigning a unit the same numerical SL as a boundary, or by violating strong directional constraints derived from locked relationships. Consequently, the admissibility of a candidate position for one unit may depend on the positions assigned to the other units in the model. If no unique reference can be established, alternative positions are retained rather than imposing an automatic assignment.

Intrusive units are treated separately because their structural position is generally controlled by their intrusive contacts. When an IU is associated with boundaries classified as intrusive, these contacts provide potential reference levels, with conformable intrusive contacts taking priority over unconformable ones. When a unique reference contact with known SL can be identified, the IU is positioned within the adjacent interval at numerically lower SL values, corresponding to a relatively higher structural position. This convention reflects the cross-cutting relationship between an intrusion and its host rocks, establishing a relative structural ordering from the host-rock domain, across the intrusive contact, towards the intrusive body. This ordering is intended as a topological reference within the STM, rather than a representation of the complete emplacement, crystallisation, and cooling history of the intrusion. When several intrusive contacts are present and no unique reference can be established, alternative positions remain unresolved rather than imposing an arbitrary ordering.

When several globally compatible configurations remain equally supported, all equivalent solutions are retained. Such ambiguities may arise either from the interaction among several admissible unit positions or from units whose STM relationships do not provide sufficient information to distinguish their relative positions, as may occur for tectonic units in duplex structures (Fig. 3) or stratigraphic units showing facies heterotopy. In these cases, topology alone may be insufficient to establish a unique relative order, even though an internal boundary or additional geological interpretation may constrain the admissible alternatives. The topology-constrained assignment of SL is therefore intended to support geological reasoning rather than replace interpretative decisions.

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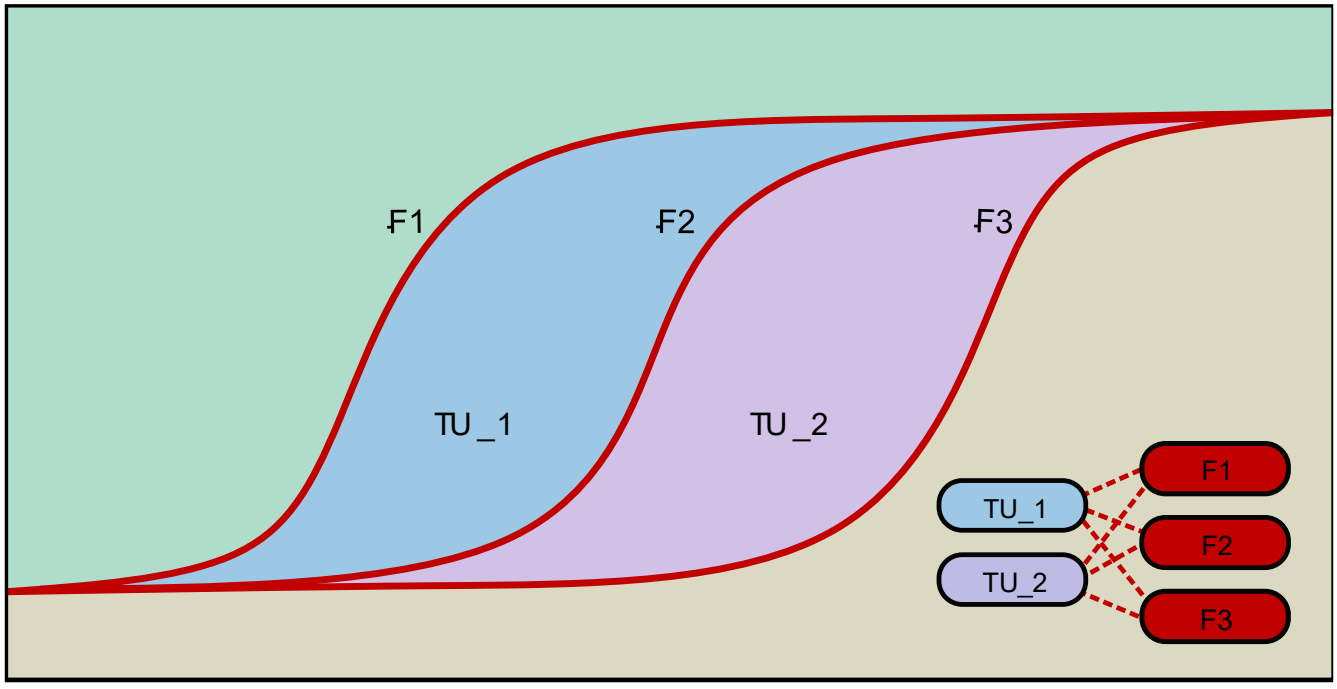


Figure 3: Example of a duplex where the two slices present the same topological signature S(u) at the section scale. On the right a topological graph shows the topological connection between the two units and the bounding faults (F1, F2 and F3). These units remain topologically indistinguishable without an input from the interpreter.

3.3 Topological matching and geological attribution

The PSC operates on the topology of the interpreted geological boundaries and assigns geological meaning to the resulting regions by comparing their local boundary relationships with the global topological signatures *S(u)*.

The geometrical partition may consist of closed polygons in 2D cross-sections or connected volumetric regions in 3D models. In both cases, the boundaries delimiting each region provide the local topological information required for geological attribution. For a generic region *r*, the PSC identifies the geological boundaries contributing to the regional boundary ∂r and defines the observed local signature:

$$L(r) = \{b \in B \mid b \; contributes \; to \; \partial r\}. \quad (5)$$

Only boundaries contributing to the geometrical subdivision are considered in the local signature, whereas structural discontinuities that do not delimit distinct regions are excluded. A match is considered exact when:

$$L(r) = S(u), \quad (6)$$

whereas a partial match is admissible when:

$$L(r) \subsetneq S(u), \quad |S(u) \backslash L(r)| \leq \mathrm{M}, \quad (7)$$

where the subset $|S(u) \backslash L(r)|$ represents the set of expected boundaries missing from the local signature, and M is the user-defined Max missing threshold, limiting the cardinality of this set. This threshold is introduced to preserve the consistency of the assignment algorithm: when the available evidence is insufficient, leaving a region unassigned is preferable to making an

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unreliable assignment. Missing expected boundaries can therefore be tolerated within the specified threshold. Conversely, the presence of an observed geological boundary that is incompatible with a candidate signature invalidates that candidate.

This distinction is particularly relevant because an individual region may expose only part of the complete topological signature of its corresponding geological unit. Some boundaries may fall outside the selected domain, or simply not intersect the considered geometrical region. Moreover, repeated occurrences of the same geological unit may exhibit different subsets of its global topological signature, for instance as a result of tectonic duplication (Sect. 3.4).

Assignments are performed hierarchically according to the information content of the observed signatures. Unique exact matches, as in Eq. (6), are processed first and assigned the CERTAIN status, as they represent the most constrained correspondence between a local region and an STM unit.

The remaining regions are evaluated using admissible partial matches. Partial signatures are ranked from the most informative to the least constrained. Regions preserving a larger and more discriminating subset of their expected STM boundaries are therefore evaluated first.

A unique admissible partial match, satisfying Eq. (7) is classified as LIKELY.

When more than one STM unit remains compatible with a local signature with equivalent topological support, the attribution is classified as AMBIGUOUS. Regions for which no admissible candidate exists, including cases in which the number of missing expected boundaries exceeds Max missing, are classified as UNASSIGNED.

These categories describe the outcome of the topological matching procedure rather than probabilities or measures of geological certainty.

3.4 Structural repetitions and topological ambiguity

A geological unit may occur more than once in the model domain because of structural processes (e.g. fault repetition) or due to the geometrical intersection with a cross-section. The PSC therefore treats the quality of a topological match and the occurrence of a repeated unit as two separate properties.

Once a unit u has received a unique CERTAIN or LIKELY assignment, any additional area compatible with the same STM unit is evaluated as a potential repeat (according to the Max missing threshold). If the two occurrences are adjacent, repeat validation examines whether their shared geological boundary is conformable with respect to the unit. Repetition across a fault, or another boundary unconformable with respect to the unit, is considered topologically admissible. Conversely, a conformable boundary cannot separate two distinct occurrences of that same unit, as this would violate the oriented-topological relationships defined in the STM. In this case, the additional assignment is therefore rejected as a conflict, and the remaining candidates are evaluated. Topologically admissible repeats retain the status associated with their matching quality: CERTAIN for an exact match and LIKELY for a partial match.

Units characterised by identical STM signatures cannot be distinguished by the initial PSC matching procedure unless additional geological information is explicitly introduced. This also applies to units sharing the same global signature $S(u)$ but differing in their conformable and unconformable relationships, since conformability is not included in the initial signature

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comparison. Ambiguity is treated independently from repetition. If the local signature of a region is compatible with more than one STM unit with equivalent topological support (Fig. 3), the result is classified as AMBIGUOUS. The previous assignment of one of the candidate units elsewhere in the model does not, by itself, resolve the ambiguity. Even when a provisional attribution is required for computational purposes, the underlying geological ambiguity remains unresolved. Alternative assignments therefore remain traceable and require validation by the interpreter.

4 Implementation in PZero

The applications presented in this work were implemented within PZero, an open-source Python platform for explicit and implicit (the latter based on LoopStructural, https://loop3d.org/LoopStructural; Grose et al., 2021) 3D geological modelling, interpretation, and data management (Bistacchi et al., 2021; Monti et al, 2024). PZero provides a common project environment in which geological entities, geometries, attributes, and their metadata can be stored, visualized, edited, and processed. Its graphical interface is based on Qt, while geological objects and 3D visualization rely on VTK data structures. Project information is organised through dedicated collections and tabular structures, while PyVista provides higher-level access to VTK data handling and visualisation.

For the three-dimensional meshing workflow, PZero is directly integrated with PyMeshIt, an open-source Python workflow based on the approach originally developed for the C++ MeshIt software (Cacace and Blöcher, 2015; Hussain et al., 2026). In this configuration, geological surfaces and their metadata can be transferred directly from the PZero project and used to construct watertight piecewise linear complexes (PLCs) and conforming tetrahedral meshes. Of particular relevance to the present work is the preservation of geological surface identity during the construction and tetrahedralization of the PLC, which allows the resulting volumetric partition to retain its correspondence with the original geological interpretation (Hussain et al., 2026).

Within this software framework, the STM is integrated directly into the PZero project structure through a dedicated specialised type of custom table and relationship metadata linked to the geological entities and attributes already defined in the project. The geological legend provides information for importing STM boundaries, while dedicated tools support unit management and the editing of topological relationships. As summarised in Fig. 4, the implementation is organised into three connected components: (1) STM data management and graph-based editing, (2) PSC analysis of geological cross-sections, and (3) volumetric PSC analysis within the PZero–PyMeshIt workflow. Both PSC workflows access the same STM representation,

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while retaining dimension-specific procedures for constructing and analysing the geometrical partition. In addition, material seeds generated from geological cross-sections can optionally be transferred to the three-dimensional meshing workflow.

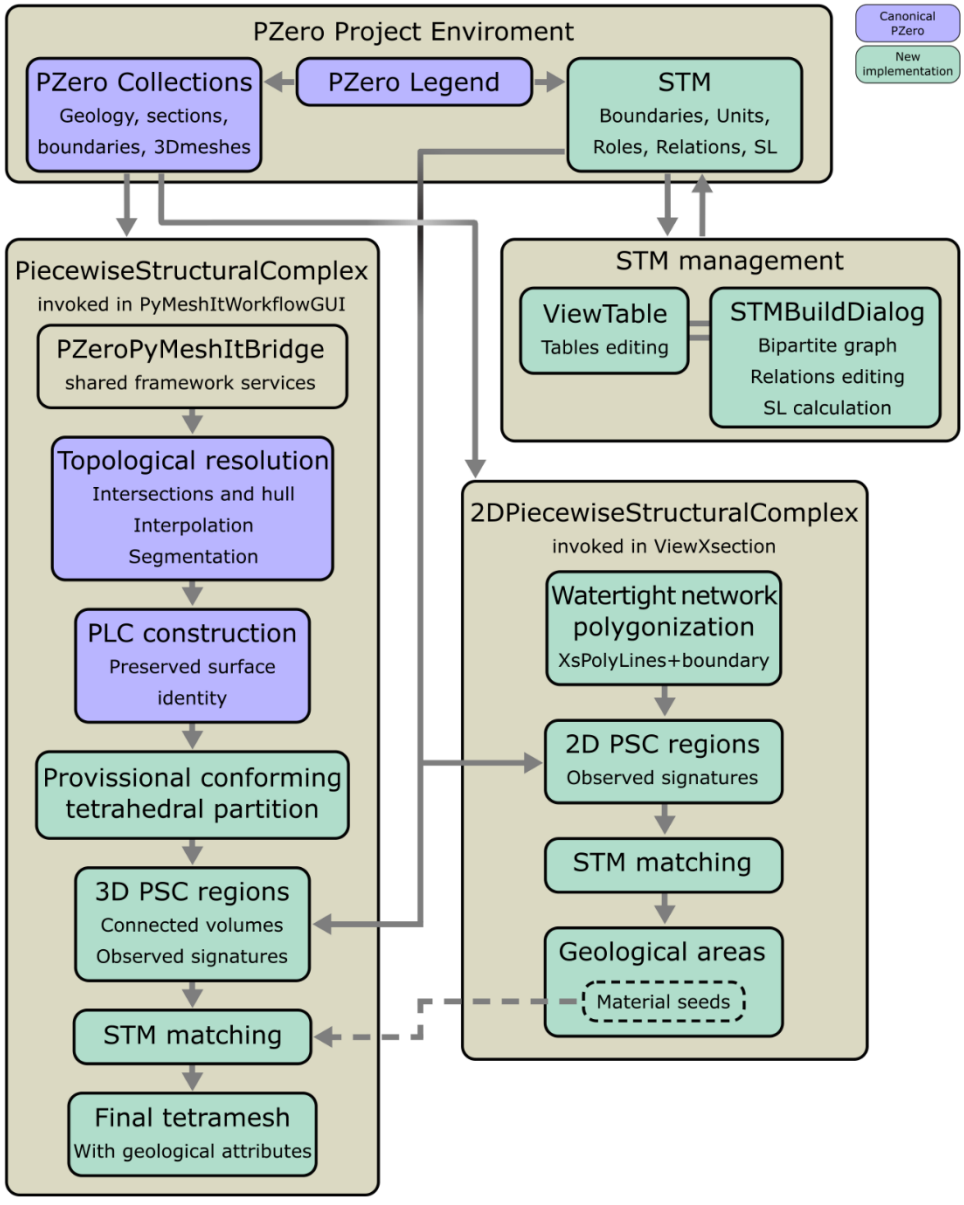


Figure 4: Architecture and data flow of the STM–PSC implementation in PZero. The STM is constructed from the shared geological legend and is managed through tabular and graph-based interfaces. The geological collections provide the geometries used by the modelling workflows. The same STM representation is accessed by the 2D cross-section and 3D PZero–PyMeshIt workflows, which derive local PSC regions and observed topological signatures before STM-based matching and geological assignment. Material seeds generated in 2D can optionally be transferred to the 3D workflow.

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4.1 STM data structures and geological entity identity

STM data are organised into two coordinated tables, dedicated to boundaries and geological units, respectively, and complemented by metadata describing their topological relationships.

The *Boundaries* table contains the geological feature label (Feature), its geological role (Role), its SL (stored as Level), and the units connected to it. Allowed roles are derived from the PZero geological legend and filtered according to the surface entities used by STM, including top, base, fault, tectonic, intrusive, and unconformity. An additional role is the special model_boundary, which is used to represent the geometrical limit of the model. Unlike geological boundaries, the Model Boundary is not assigned a geologically meaningful SL. Internally, its Level is set to $-\infty$ as a sentinel value for graphical ordering, without contributing numerical constraints to the automatic SL calculation.

Similarly, the *Units* table contains the unit name (Feature), the unit role (TU, SU, IU, or SD), its SL, the conformable and unconformable boundaries associated with the unit, and an optional series of Domain_n fields. Conformable and unconformable relationships are stored separately in the Units table and in the associated STM metadata, whereas the Boundaries table contains the overall list of connected units without distinguishing their conformability. Locked conformable relationships are maintained as additional metadata. These representations are synchronised to preserve the consistency of the STM graph.

Within the STM, geological boundaries are identified by their Feature labels rather than by the unique identifiers (UIDs) of individual geometrical objects. Consequently, multiple geometrical objects sharing the same Feature and Role can represent different portions of a single conceptual boundary without generating separate nodes in the STM graph. The geological Role is retained as an attribute and can support the association between STM boundaries and geometrical surfaces, but it does not constitute part of the topological identifier.

STM boundaries are imported from the geological legend associated with the PZero geological collection, rather than directly from individual geometrical objects. The legend provides their Feature, Role, SL, and colour attributes. Boundaries that are not represented by existing VTK objects can be added manually, allowing the STM framework to include conceptual elements that have not yet been modelled, reflecting the a priori nature of STM. Similarly, the model boundary can be represented either by an imported box from the boundary collection, or by defining a conceptual model extent.

The optional Domain_n fields store geological group memberships as unit metadata. Neither the SL calculation nor PSC signature matching uses domain membership as a topological constraint.

The STM tables and associated relationships are saved within the PZero project, allowing the graph to be reconstructed when the project is reopened. The core tabular STM information can also be exported independently in JSON format, providing a transferable representation of geological units, boundaries, and their topological relationships.

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4.2 SL solver and interactive ambiguity resolution

If the SL of a unit is not manually defined in the table, the unit is initially displayed in the graph without an SL-based position. Once the graph has been constructed, the calculation can be initiated from the STM Builder, using the boundary levels, geological roles, and unit–boundary relationships stored in the STM tables and metadata, while existing manually defined SL values can either be retained or overwritten during the calculation.

At execution, the solver retrieves the numerical SL values of the geological boundaries and the associated conformable, unconformable, and locked relationships. Candidate values are generated and evaluated according to the constraints described in Sect. 3.2, producing a set of globally admissible STM configurations. Figure 5 summarises the corresponding decision workflow, distinguishing the dedicated IU procedure from the other unit types.

The software presents one ambiguous unit at a time and restricts the available SL values to those occurring in the configurations that remain compatible with the previous choices. Each user selection filters the global solution set and updates the alternatives available for the remaining units. Units that consequently acquire a unique SL are resolved automatically, and further user intervention is requested only for the next unit that remains ambiguous. Although choices are presented individually, they therefore remain constrained by the compatibility of the complete STM configuration.

Units for which no admissible SL can be determined automatically can be assigned manually. These values are stored as unit-specific overrides and take precedence over subsequent automatic results when the user chooses to retain them. Values generated during the ambiguity-resolution sequence are committed only after the entire sequence has been completed; if the procedure is cancelled, partial decisions are not retained.

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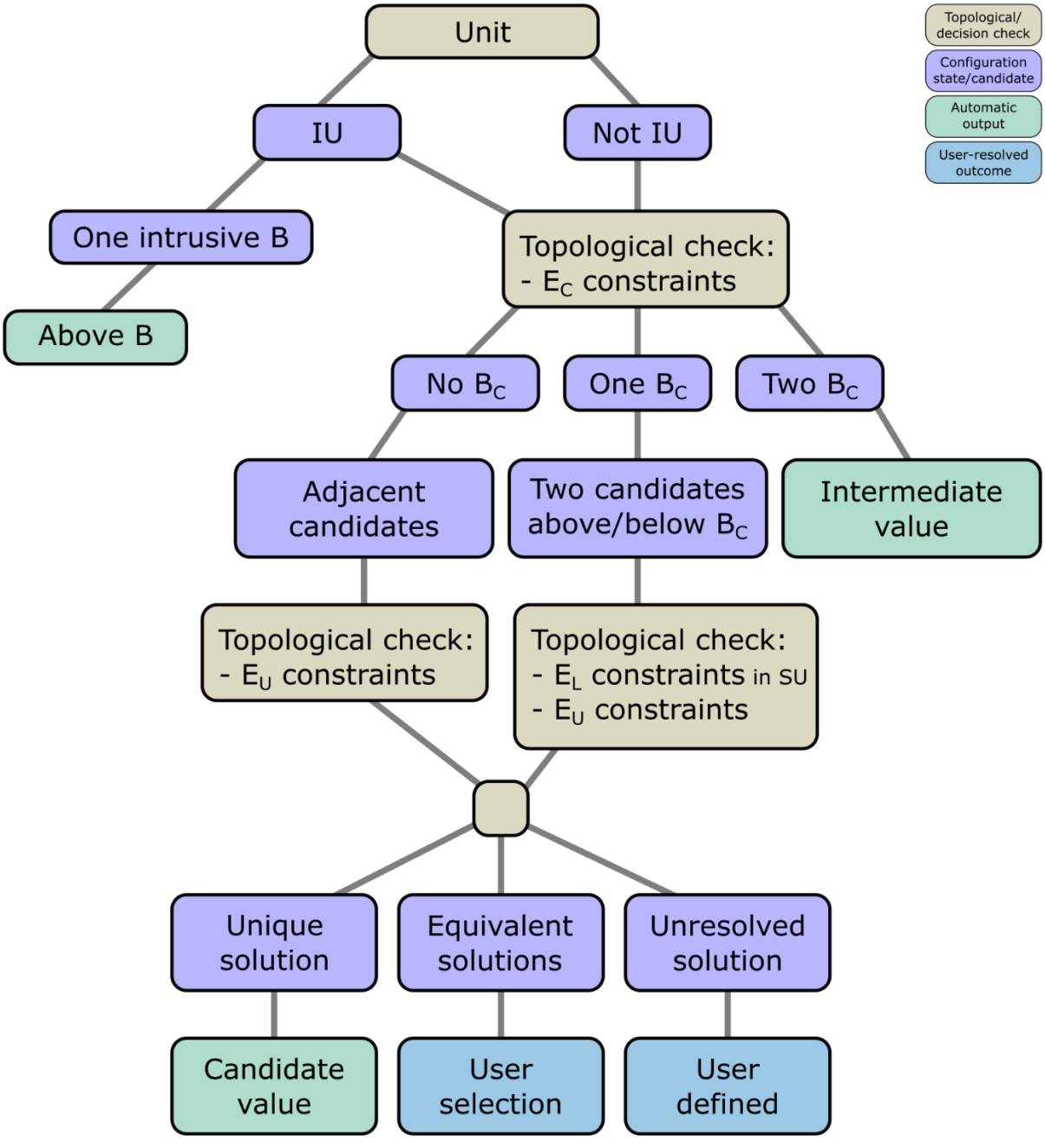


Figure 5: Decision workflow for topology-constrained Structural Level (SL) calculation in the PZero STM Builder. Candidate SL values are generated according to the geological unit type and its relationships with conformable, unconformable, and intrusive boundaries. The candidates are evaluated against the STM topological constraints to identify globally compatible configurations. Where multiple solutions remain admissible, the user selects among the alternatives; units without a sufficiently constrained solution can be assigned an SL manually.

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4.3 PSC matching

The PSC matching procedure is implemented in both the 2D cross-section and 3D volumetric workflows using the same topological attribution criteria (Sects. 3.3–3.4). Once the geometrical partition has been reconstructed, each region is associated with the geological boundaries delimiting it and, where applicable, with its topological relationships to neighbouring regions. The procedures used to obtain this information differ between 2D and 3D and are described in the following sections.

The matching routine constructs and prioritises the admissible candidate list according to the criteria defined in Sect. 3.3 and described in Fig. 6. Before an attribution is recorded, candidates are filtered against repeat conflicts using the region adjacency information reconstructed by the corresponding 2D or 3D workflow (Sect. 3.4). If no admissible candidate remains, the region is classified as UNASSIGNED. The resulting attribution and matching status are retained for subsequent geometrical processing and material assignment. Where computational operations require a provisional unit attribution for an ambiguous region, this does not replace the AMBIGUOUS classification or eliminate the need for geological interpretation.

4.3.1 PSC in 2D cross-sections

The 2D PSC workflow operates on the XsPolyLines associated with a geological cross-section in PZero. Before any geological attribution is attempted, the interpreted XsPolyLines network is tested for topological consistency together with the frame of the cross-section or the intersection of the model boundary. The network is required to form a complete sealed planar subdivision in order to generate polygons as triangulated surfaces (TriSurf). The procedure checks for dangling segments, incomplete cuts, invalid rings, and insufficient boundary coverage. These conditions indicate that the interpreted XsPolyLines do not completely partition the selected section domain. If the network is not watertight, polygonization is considered unreliable and PSC construction is interrupted.

For a valid network, polygonization partitions the cross-section into a set of closed areas represented by TriSurf geometries. For each polygon, the algorithm identifies the contributing XsPolyLine segments and retrieves their geological Feature labels. Multiple segments associated with the same Feature contribute only once to the local topological signature. The resulting

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signatures are passed to the matching procedure described in Sect. 4.3, together with the polygon adjacency information required for repeat validation.

Following geological attribution, the resulting polygons retain their assigned geological units and matching statuses. The workflow also generates reference points as XsVertex objects, which can be used as material seeds in the subsequent 3D workflow (Sect. 4.3.3).

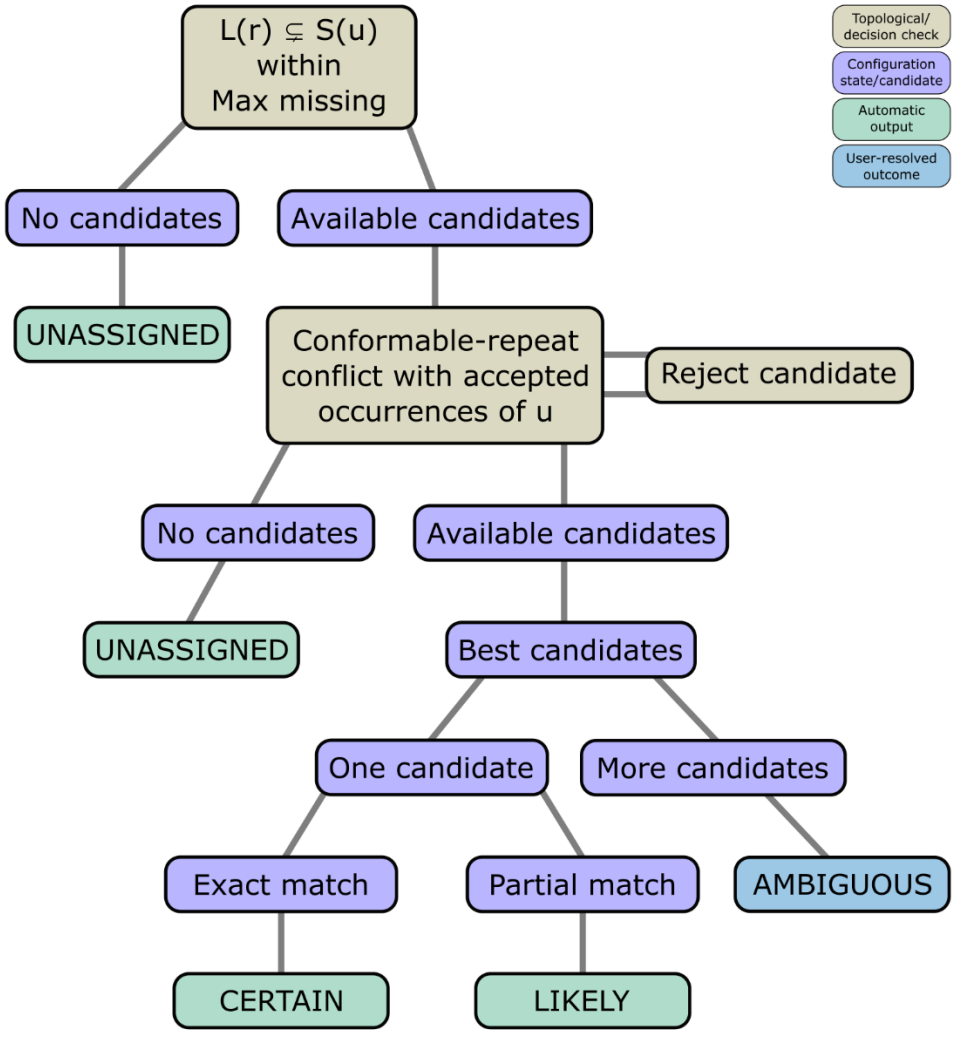


Figure 6: Decision workflow for PSC topological matching and structural repetition validation in 2D and 3D. The local topological signature of each reconstructed region is compared with the global unit signatures derived from the STM graph. Candidate units are identified through exact or partial matching within the user-defined Max missing threshold. Candidates producing topologically inconsistent repetitions across boundaries conformable with respect to the assigned unit are rejected. The remaining candidates are evaluated according to match quality and uniqueness, resulting in CERTAIN, LIKELY, AMBIGUOUS, or UNASSIGNED classifications.

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4.3.2 PSC in 3D tetrahedral meshes

During the final stage of the PyMeshIt workflow, triangulated geological surfaces are assembled for the generation of the final tetrahedral mesh (Hussain et al., 2026). Material IDs can then be assigned to the different geological regions of the model. To support this operation, the 3D PSC reconstructs a provisional volumetric partition and generates internal seed points for subsequent material attribution.

The procedure first associates the geological surfaces loaded in PyMeshIt with the corresponding STM boundaries. Surfaces defining the external model domain require specific treatment. Although the faces of the bounding box are handled as separate geometrical objects in PyMeshIt (Hussain et al., 2026), they are normalised to a single STM entity, Model Boundary. Consequently, a geological unit intersecting several faces of the external domain records only one external boundary in its topological signature.

The volumetric partition is reconstructed through a provisional tetrahedralisation of the loaded surfaces using TetGen. The resulting mesh is retained and can be reused when PSC parameters are modified, avoiding unnecessary repetition of the tetrahedralisation step.

The provisional tetrahedral mesh is then analysed as a connectivity problem. Two neighbouring tetrahedra belong to the same volumetric region when their shared face is not part of an input geological surface, whereas geological surfaces interrupt tetrahedral connectivity. The connected components obtained from this procedure therefore represent the volumetric regions defined by the interpreted geological model. However, surfaces that do not interrupt tetrahedral connectivity and therefore do not generate distinct PSC regions (e.g. minor faults) are not interpreted as unit boundaries and do not contribute to the local topological signatures, although they may be retained as internal discontinuities within the tetrahedral mesh.

For each reconstructed region, the PSC records its constituent tetrahedra, delimiting geological surfaces, neighbouring regions, and separating interfaces, providing the information required by the common matching and repeat-validation procedure described in in Sect. 4.3.

An internal seed is generated for each reconstructed region for subsequent material attribution. Rather than using the centroid of the entire region, which may fall outside strongly concave geometries, the algorithm evaluates the tetrahedra belonging to the connected component: for each tetrahedron, its incenter and corresponding inscribed-sphere radius are calculated, and the incenter associated with the largest radius is selected as the regional seed. The resulting point is therefore guaranteed to lie inside the region and preferentially maximises its distance from the surrounding tetrahedral faces.

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4.3.3 Integration between 2D and 3D PSC workflows

Although the 2D and 3D PSC procedures operate independently on section and volumetric geometries, additional tools allow information to be transferred between the two workflows. As described in Sect 4.3.1, the 2D polygonization procedure generates a reference seed as an XsVertex for each reconstructed polygon. These seeds can be imported directly into PyMeshIt while preserving their geological attribution, when available, providing predefined material seeds for subsequent tetrahedral meshing. This creates a direct connection between geological interpretation in cross-section and construction of the three-dimensional model (Fig. 4). This transfer allows geological attribution to be controlled directly in cross-section, reducing the need for manual seed placement in the 3D model. However, a single cross-section may not intersect every disconnected volumetric region, so additional cross-sections or manually defined material seeds may be required to complete the attribution. Additional geometrical information can be introduced in models where interpreted geological boundaries extend above the present-day topography. This subdivision is performed after PSC matching, and the resulting portions inherit the geological attribution of their parent polygons. Portions located above the topography can be identified as eroded occurrences, whereas those below represent the preserved subsurface configuration. Eroded occurrences receive dedicated Feature labels with the suffix _eroded and separate material seeds. In PyMeshIt, these seeds can either retain separate material labels derived from their original geological units or be assigned to a single virtual material named eroded. This option merges material attribution rather than the underlying geometries. The eroded materials are handled independently of ordinary STM signature matching; consequently, the topographic subdivision does not modify the original STM signatures or the geological attribution established before the cut.

4.4 Graphical tools and user interaction

The STM data structures described in Sect. 4.1 are managed through dedicated tabular interfaces and the STM Builder, which allow geological units, boundaries, and their relationships to be created and modified interactively. When a boundary represents a reference surface for a unit, as commonly occurs for SU tops or IU intrusive contacts, the Generate units command allows the creation of the corresponding unit with a locked conformable relationship (E_L). The initial unit role is automatically proposed according to the role of the surface: top and base boundaries initially generate an SU, intrusive boundaries an IU, and fault or tectonic boundaries a TU. However, this classification can subsequently be modified by the user. Units without a representative surface can be added independently and subsequently connected to the boundaries defining their topological signature.

Relationships between units and boundaries are edited through the STM Builder, which provides a graphical representation of the bipartite graph, with units and boundaries displayed in separate columns. These are ordered according to their SL (with values decreasing upwards), while the graphical elements retain the colours defined in the geological legend or during tables' compilation. Conformable and unconformable relationships are represented using different line styles (respectively continuous or dashed) and can be added, removed, or reclassified directly in the Builder, whereas locked relationships are preserved.

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During editing, the STM tables are automatically updated, keeping the graphical representation and the topological information synchronised.

In the Builder, domains visually group the units assigned to them and can be used to select and manage multiple units in a single step, e.g. connecting basement TUs to a regional unconformity (higher-order boundary). These operations are applied to the individual units belonging to the selected domain, allowing relationships to be edited collectively without introducing additional nodes or connections at domain level.

The STM Builder also provides access to the automatic SL calculation and its interactive ambiguity-resolution procedure, described in Sect. 4.2.

The PSC tools provide dedicated controls for the construction and attribution of geological regions. In cross-sections, the user can define the partitioning domain using either the section frame or an available model boundary, select the XsPolyLines to be included, and optionally use a DEM-derived topographic trace to subdivide the resulting areas.

The Switch PSC areas tool is primarily intended to correct inverted geological assignments between ambiguous regions. The user selects the polygons to be exchanged, including possible eroded occurrences, and the tool swaps their Feature and Role attributes, automatically updating the corresponding XsVertex seeds.

In PyMeshIt, a dedicated PSC button activates the volumetric attribution procedure and opens a results table, allowing the user to inspect the assignments, switch ambiguous geological attributions, or import material seeds generated from PZero cross-sections. These graphical operations complement the 2D and 3D procedures described in Sect. 4.3.

5 Applications in benchmarks

The STM–PSC implementation is evaluated through six benchmark cases, comprising three synthetic cross-sections, one synthetic 3D model, and two geological models derived from real datasets. The examples assess topology-constrained SL calculation, PSC matching, and geological attribution across two- and three-dimensional geometries.

5.1 Cross-section benchmarks

The three synthetic cross-sections progressively examine the effects of incomplete boundary exposure, structural repetitions, and ambiguous topological relationships on SL calculation and polygon attribution.

5.1.1 Cross-section 1

This synthetic cross-section represents a simple monocline composed of four SUs (SU1-4) separated by continuous and conformable stratigraphic boundaries (Fig. 7). At the model scale, the higher SU3 and SU4 are also truncated by an unconformity (Unc1), which is therefore part of their global topological signatures (Fig. 7b). However, Unc1 does not intersect the selected cross-section. Consequently, the local signatures of SU3 and SU4 contain only a subset of their expected STM boundaries, providing a simple test of the PSC partial-matching procedure.

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The same configuration also provides a straightforward test of the automatic SL calculation for units. SU2 and SU3 are each associated with two conformable boundaries, one of which is linked through a locked relationship. SU1 has only one conformable boundary, but its locked relationship with topSU1 provides a strong directional constraint. SU4, conversely, is associated with one non-locked conformable boundary and one unconformable boundary; nevertheless, the solver assigns the expected SL within the resulting STM configuration.

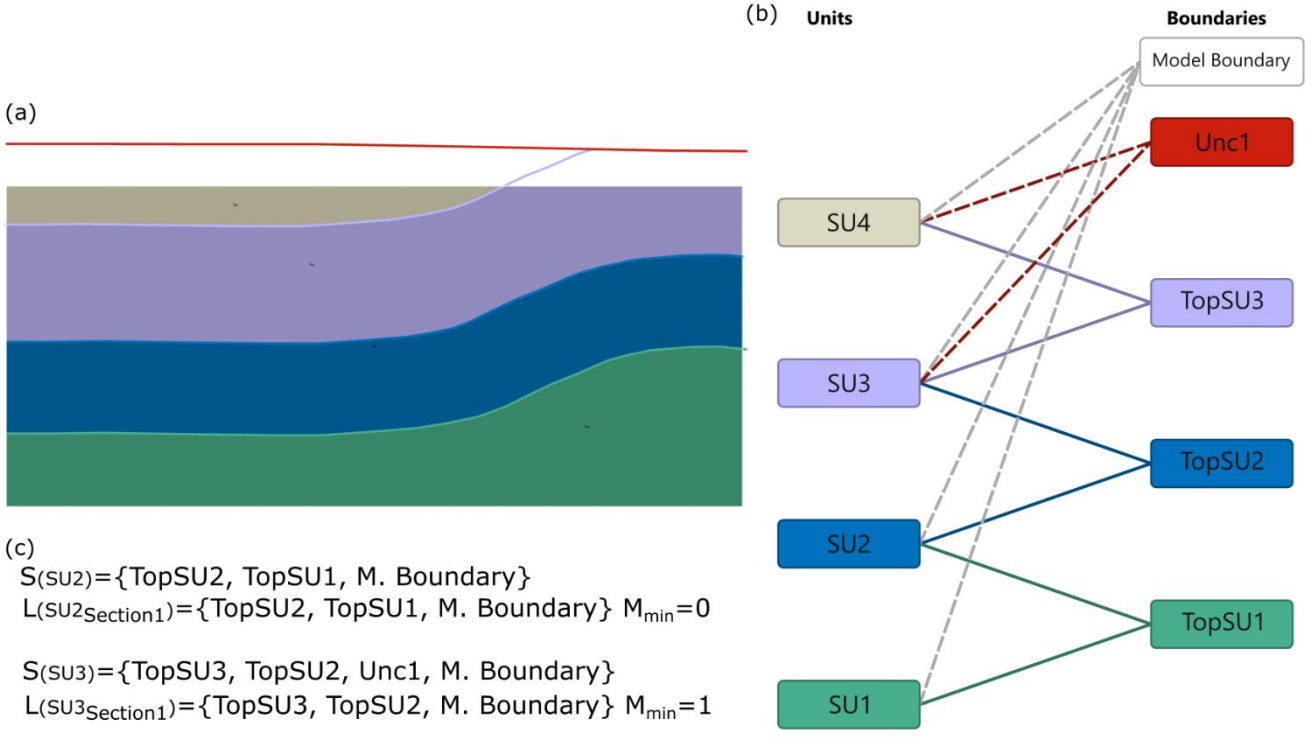


Figure 7: The cross-section 1 after polygonization of its XsPolylines (a) and the STM graph exported from PZero (b), where conformable relations E_C and unconformable relations E_U are represented respectively by continuous and dashed lines. Part of the boundary TopSU3 and the Unc1 are shown outside from the section frame used for polygonization, resulting for both SU3 and SU4 to have a local topological signature incomplete (1 missing boundary). Seeds are automatically generated during polygonization and plotted as XsVertex. (c) Examples of global and local topological signatures: SU2 exhibits an exact match, whereas SU3 exhibits a partial match with a minimum Max missing value required for an admissible match M_{min}=1.

5.1.2 Cross-section 2

This synthetic cross-section represents an extensional system developed within a pre-existing tectonic unit TU1 and controlled by two syn-sedimentary faults, F1 and F2. SU5 and SU6 were deposited during fault activity, filling the resulting horst-and-graben geometry and are separated by a continuous and conformable stratigraphic boundary. Their succession rests on Unc3, which is displaced by both faults. The extensional system is subsequently truncated by the younger unconformity Unc2, which cuts SU6 and seals both faults. A younger post-extensional stratigraphic unit, SU7, is deposited above Unc2 (Fig. 8a).

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The automatic SL calculation resolves the structural position of the more strongly constrained units, whereas SU7 and TU1 retain multiple admissible positions because neither unit has conformable relationships that sufficiently constrain its structural position. Excluding the Model Boundary, TU1 is connected only to Unc3 and the two faults through unconformable relationships, whereas SU7 is connected only to Unc2, also unconformably. The algorithm therefore retains the two structural intervals adjacent to Unc2 (SL equal to 1) as admissible candidates, corresponding to SL values of 0.5 and 1.5. The user selects the geologically consistent value, SL = 0.5. Once this choice has filtered the set of globally compatible configurations, TU1 remains compatible with three alternative positions, at SL = 1.5 and 2.5, related to the faults, and 5.5. As its topology does not provide sufficient constraints to discriminate automatically among these intervals, a second user selection is required, with SL = 5.5 representing the geologically consistent solution according to Unc3 (SL equal to 5). These ambiguities arise because both units are only weakly constrained by the available boundary relationships, rather than from a failure of the automatic calculation. Their topological signatures define a set of admissible structural positions, but do not contain enough directional or conformable constraints to select a unique solution.

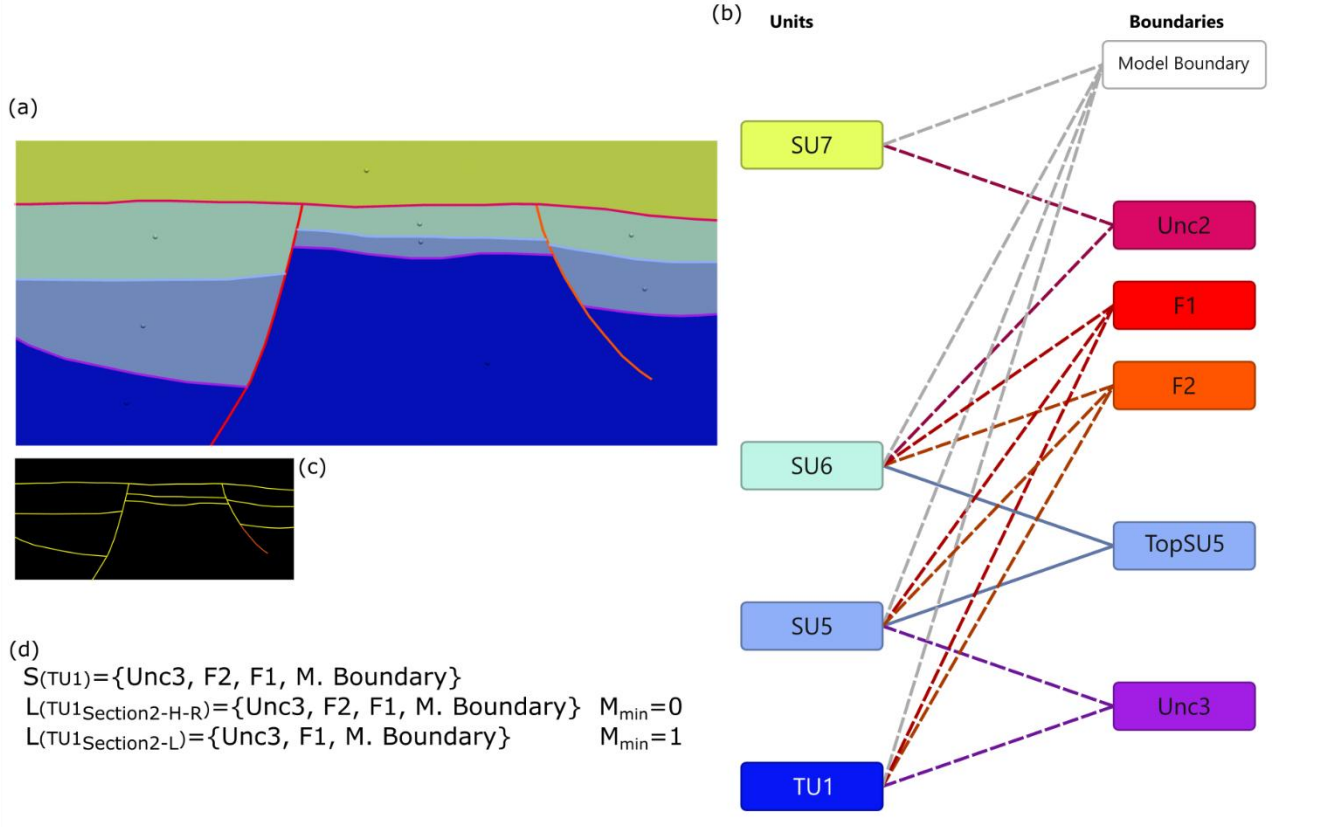


Figure 8: The cross-section 2 after polygonization of its XsPolylines (a) and the STM graph exported from PZero (b), where conformable relations E_C and unconformable relations E_U are represented respectively by continuous and dashed lines. To ensure sealed connections between XsPolyLines and the section frame, F2 has been split at the intersection with Unc3 and discarded during polygonization (c). Seeds are automatically generated during polygonization and plotted as XsVertex. (d) Examples of global and local topological signatures of TU1 in its two occurrences in section 2 (H-R: horst and right graben; L: left graben).

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In the left half-graben, the succession is completely separated from the central horst at the scale of the section (Fig. 8a). TU1 therefore occurs on both sides of F1, while SU6 is repeated and its two occurrences are directly adjacent across F1. This configuration does not generate a topological conflict because their common interface is a fault, i.e. a boundary unconformable with respect to SU6, rather than a conformable boundary that would incorrectly separate two occurrences of the same unit. SU5 is also repeated, but its two occurrences are not mutually adjacent and therefore do not require adjacency-based repeat validation.

The right half-graben shows a similar repetition of SU5, here with adjacent occurrences, and SU6 across F2, but additionally illustrates the treatment of a fault terminating within a unit. While the upper segment of F2 extends from Unc3 to Unc2 and effectively separates different section areas, its lower segment terminates within TU1. If included in the polygonization network, this lower segment would constitute a dangling XsPolyLine, causing the network to fail the preliminary watertightness check and therefore preventing PSC construction. F2 is consequently split at its intersection with Unc3: the segment between Unc3 and Unc2 is selected for polygonization, whereas the lower segment is retained in the geological interpretation as an internal discontinuity of TU1, without contributing to the PSC partition (Fig. 8c).

More generally, the SUs occurring in the right half-graben and in the horst, and the units forming the entire left half-graben preserve only partial local topological signatures relative to their global STM signatures (Max missing = 1). Different occurrences of the same geological unit may therefore expose different subsets of the boundaries contained in its global signature. These areas are consequently identified through partial matching, illustrating how the PSC can recognize repeated units even when their complete topological signature is not locally represented.

5.1.3 Cross-section 3

This synthetic cross-section introduces hierarchical geological domains and illustrates a case in which ambiguity affects both SL assignment and geological unit attribution.

The domain “Nappe 1” comprises TU2 and TU3, which are separated by the tectonic contact Tect1, conformable with respect to both units. Tect2 juxtaposes Nappe 1 against TU4, contacting both TU2 and TU3, whereas Tect3 places this assemblage against TU5. All four tectonic units belong to the higher-level “Basement” domain. The same hierarchy is expressed by the truncation relationships among boundaries. Tect2 cuts across Nappe 1, whereas Tect3 truncates both Nappe 1 and Tect2, thus defining a progressively higher-order partition at the scale considered. The structure is finally truncated upward by Unc4, which cuts TU4 and TU5 and is overlain by the younger stratigraphic unit SU8 (Fig. 9).

TU2 and TU3 have identical topological signatures: both are bounded by the same set of geological contacts, and their relationships do not provide sufficient directional information to distinguish their relative structural positions (Fig. 9b). Their ambiguity is therefore intrinsic to their topology rather than resulting from missing section information. Tect1 nevertheless provides an internal separator between the two units, allowing the solver to construct two alternative, globally compatible orderings, on either side of Tect1 (SL = 4). During the automatic SL calculation, TU2 can consequently occupy either SL =

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3.5 or SL = 4.5, while the position of TU3 is adjusted consistently with the selected alternative. In the geological interpretation represented here, TU2 is assigned SL = 4.5.

This case therefore illustrates a different type of ambiguity from those produced by weakly constrained individual units. Here, the available topology constrains TU2 and TU3 as a pair but does not determine which member occupies each of the two admissible structural positions. The user selection resolves this symmetry, after which the corresponding SL of the other unit follows automatically. The same topological equivalence also affects unit attribution in the PSC: although TU2 and TU3 share the same global signature in a potential 3D model, their local signatures differ. With Max missing ≥ 1, both regions remain compatible with both global signatures, resulting in ambiguous unit attribution that requires geological interpretation to resolve.

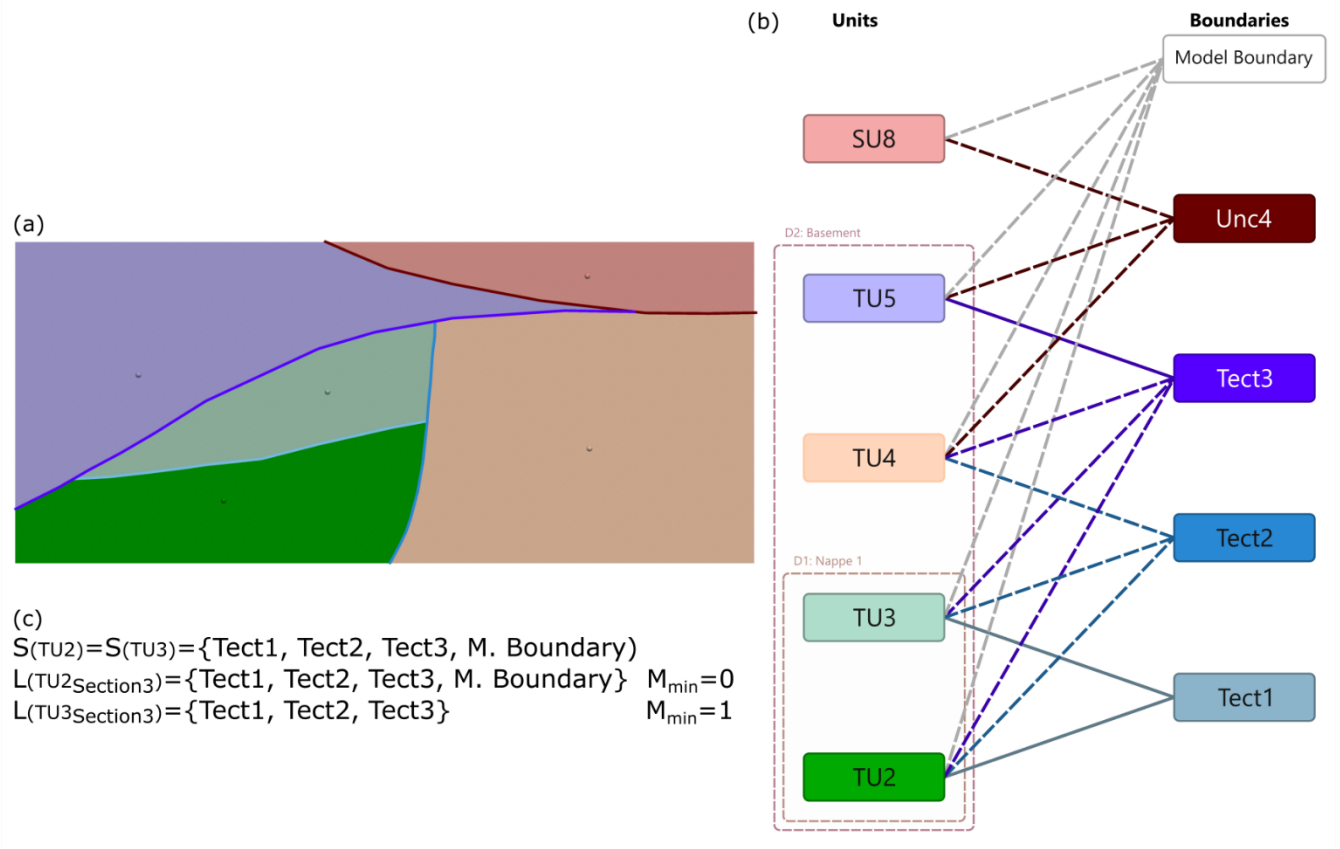


Figure 9: The cross-section 3 after polygonization of its XsPolylines (a) and the STM graph exported from PZero (b), where conformable relations E_C and unconformable relations E_U are represented respectively by continuous and dashed lines. Units are grouped into domains according to the STM table in PZero, highlighting the hierarchical position of units and boundaries. Seeds are automatically generated during polygonization and plotted as XsVertex. (c) Example of global and local topological signatures for TU2 and TU3 and their minimum Max missing values required for an admissible match.

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595

5.1.4 Cross-sections and DEM

In the cross-section PSC workflow, the topographic profile (DomXs) can optionally be used to distinguish preserved subsurface and eroded portions. Geological polygons are first generated and assigned exclusively from the geological boundary network and their STM topological signatures. The DomXs is then applied as a secondary geometrical subdivision: each
600 resulting portion inherits the attribution of the original polygon and is classified as subsurface or eroded according to its position relative to the present-day topographic surface. Separate seeds are generated for each portion and can subsequently be transferred to PyMeshIt for 3D material assignment (as described in Sect. 4.3.3). Figure 10 shows the effect of applying a topographic profile to the synthetic cross-sections 2 and 3. The geological units are subdivided into subsurface and eroded polygons. Subsurface polygons retain their original STM colours, whereas eroded occurrences are displayed using lighter
605 versions of the corresponding unit colours, preserving their geological identity while visually distinguishing them from the subsurface portions.

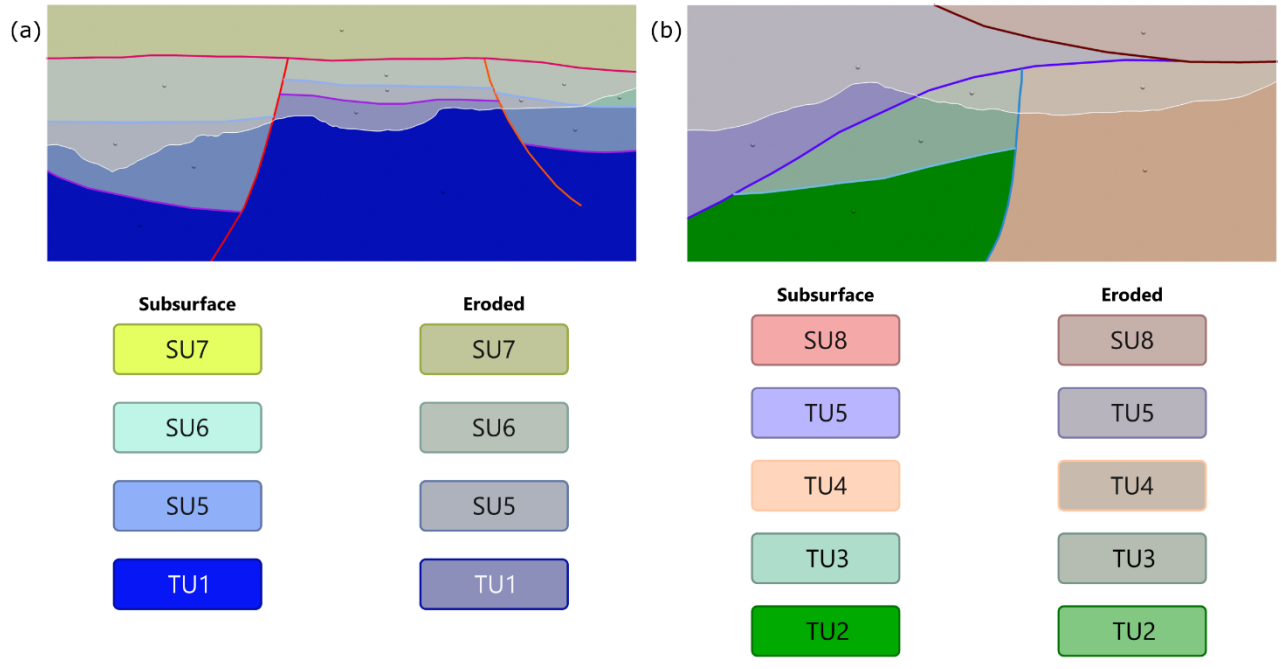


Figure 10: Synthetic cross-sections 2 (a) and 3 (b) after polygonization of the XsPolyLines, including the DomXs topographic profile. The corresponding colour legends are shown below, distinguishing subsurface from eroded portions. Seeds for both portions are
610 **automatically generated during polygonization and represented as XsVertex. For visualization purposes, eroded portions can also be hidden from the cross-section display.**

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5.2 Three-dimensional benchmarks

The three-dimensional benchmarks focus on volumetric partitioning and material attribution, examining the effects of geological complexity, topographic constraints, and internal structural discontinuities.

5.2.1 Synthetic 3D model

This synthetic 3D model comprises four tectonic units (TU0–TU3) included within the "Basement" domain. The units are sequentially juxtaposed by three tectonic contacts, with Tect1 separating TU0 from TU1, Tect2 separating TU1 from TU2, and Tect3 separating TU2 from TU3. TU0 is intruded by pluton IU2 through the intrusive contact Int2. Int2 is confined to TU0 and does not cross Tect1, consistently with its relative position preceding Tect1 in the STM ordering. A second intrusion, IU1, cuts TU1, TU2, and TU3 through Int1, cross-cutting both Tect2 and Tect3. The entire basement assemblage is subsequently displaced by Fault1, a sinistral fault with a reverse component, approximately transverse to the main structural trend. Fault displacement produces both adjacent and non-adjacent repetitions of the basement units, while TU0 and IU2 are absent from one fault block. Int1 is also not exposed in this block, representing a geometrically deeper contact in the synthetic configuration. Finally, the basement is truncated by the unconformity Unc1 and overlain by SU1 and SU2. Top1 represents the top of SU1 and is conformable with respect to both adjacent stratigraphic units (Fig. 11-12).

The automatic SL calculation correctly resolves most units (Fig. 11d), but TU0 requires manual correction: since TU0 is conformable with Tect1, and Int2 (with an higher SL value) also belongs to its topological signature, the automatic procedure identifies an admissible position between the two boundaries. However, this position is inconsistent with the relative age relationship imposed by intrusion: IU2 intrudes TU0 along Int2 and is therefore younger than its host unit. TU0 must consequently occupy a numerically higher SL, corresponding to a structurally lower and relatively older position than Int2. Its SL is therefore manually reassigned, highlighting the distinction between a configuration that is topologically admissible and one that is geologically consistent. Furthermore SU1 and SU2, despite having the same topological signature, do not generate an SL ambiguity because the locked conformable top relationship between SU1 and Top1 provides an additional directional constraint.

Three representative cross-sections were extracted from the synthetic 3D model to evaluate how section orientation and local boundary exposure affect PSC attribution (Fig 11-12a). Section 1 (Fig. 11a) samples the hanging-wall block, where the geological units are generally well constrained; a Max missing value of 2 is sufficient to assign the complete section, with TU2 representing the least complete local signature because two relationships expected from the global STM signature are not represented at section scale (Fault 1 and the model boundary). Basement and intrusive units are consequently assigned through partial matching and classified as LIKELY. Section 3 (Fig. 11c) samples the footwall block and provides a more incomplete representation of the global topology. In particular, the local signature of TU1 lacks Fault1, Int1 and Tect1, requiring Max missing = 3 for its assignment; with lower thresholds, part of the basement remains unassigned. Section 2 (Fig. 11b), oriented approximately along strike, intersects both fault blocks. The three sections therefore show that the completeness of section-

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derived PSC assignments depends on which elements of the global topological signature are actually intersected by the section. In all three sections, SU1 and SU2 remain mutually ambiguous because their identical topological signatures do not provide sufficient spatial information to distinguish their corresponding polygons. The resulting polygon assignments generate section-specific XsVertex seeds that can subsequently be transferred to the 3D meshing workflow.

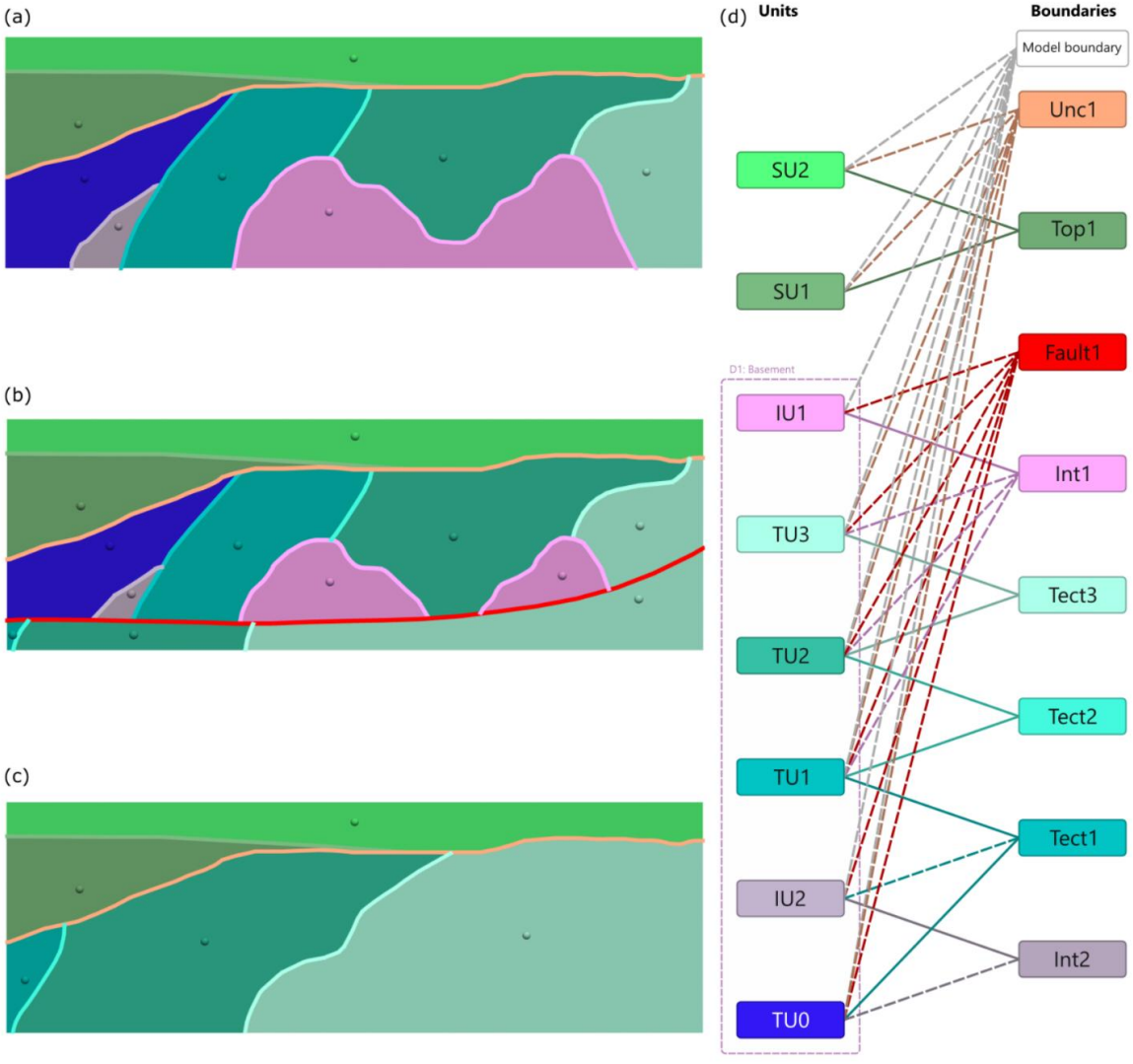


Figure 11: Representative cross-sections through the synthetic 3D model and corresponding PSC assignments. (a) Section 1, located within the hanging-wall block. All polygons are assigned with Max missing = 2; basement and intrusive units are classified as LIKELY because their local signatures preserve only subsets of the corresponding global STM signatures. (b) Section 2, oriented approximately along strike of Fault1 and intersecting both the footwall and hanging-wall blocks. The hanging-wall portion is resolved with a lower missing-boundary tolerance, whereas the footwall reproduces the more incomplete signatures observed in Section 3 and requires Max missing = 3. (c) Section 3, located within the footwall block, where TU1 lacks Fault1, Int1 and Tect1 from its local signature and therefore requires Max missing = 3; with lower thresholds, the corresponding basement polygon remains unassigned. In all sections, SU1 and SU2 remain ambiguous because they share the same topological signature. XsVertex seeds are generated from the assigned polygons and can be transferred to PyMeshIt for subsequent 3D material attribution.

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The model also provides a three-dimensional PSC test of partial topological matching and unit repetition across Fault1 in PyMeshIt (Fig. 12c). In the hanging-wall block, the basement units preserve their complete global STM signatures and are therefore correctly identified from the full set of expected boundary relationships. In the footwall block, fault displacement and the geometry of the model result in only partial representations of the same signatures. TU1 therefore represents the most incomplete case, with two expected boundaries missing from its local signature (Tect1 and Int1). Unlike the corresponding 2D section, the volumetric region retains its relationship with Fault1, reducing the number of missing boundaries from three to two. Other basement units preserve less incomplete but partly similar signatures, resulting in several potential matches during the PSC procedure. Adjacency validation is therefore essential to discriminate among these alternatives: repetitions that would place two occurrences of the same unit across a tectonic contact defined as conformable with respect to that unit are rejected as topologically inconsistent, whereas repetitions across Fault1 remain admissible because the fault represents an unconformable boundary with respect to the displaced units.

As for 2D PSC, SU1 and SU2 are affected by ambiguous assignment, since the two units remain topologically indistinguishable during 3D PSC attribution. Consequently, both assignments remain compatible with the available PSC topology and are presented as an ambiguity, allowing the user to manually swap the two unit assignments before confirming the solution. Additional topological information would remove this symmetry: for instance, the presence of a third stratigraphic unit in contact only with SU2 would provide a discriminating relationship and allow the two volumes to be assigned uniquely.

Although the 3D PSC can independently assign the model volumes from their three-dimensional topological relationships, the section-derived seeds provide an optional way to transfer expert-controlled 2D interpretations into the 3D meshing workflow. In this example, Section 2 is particularly effective because it intersects both the hanging-wall and footwall blocks and can therefore provide, in a single section, seeds for the entire basement configuration. Sections 1 and 3 provide a complementary alternative: taken together, the hanging-wall and footwall sections sample the diagnostic relationships of both blocks and allow a more complete seed-based attribution of the basement. However, the same final material attribution is obtained using either the direct 3D PSC or the section-derived seeds.

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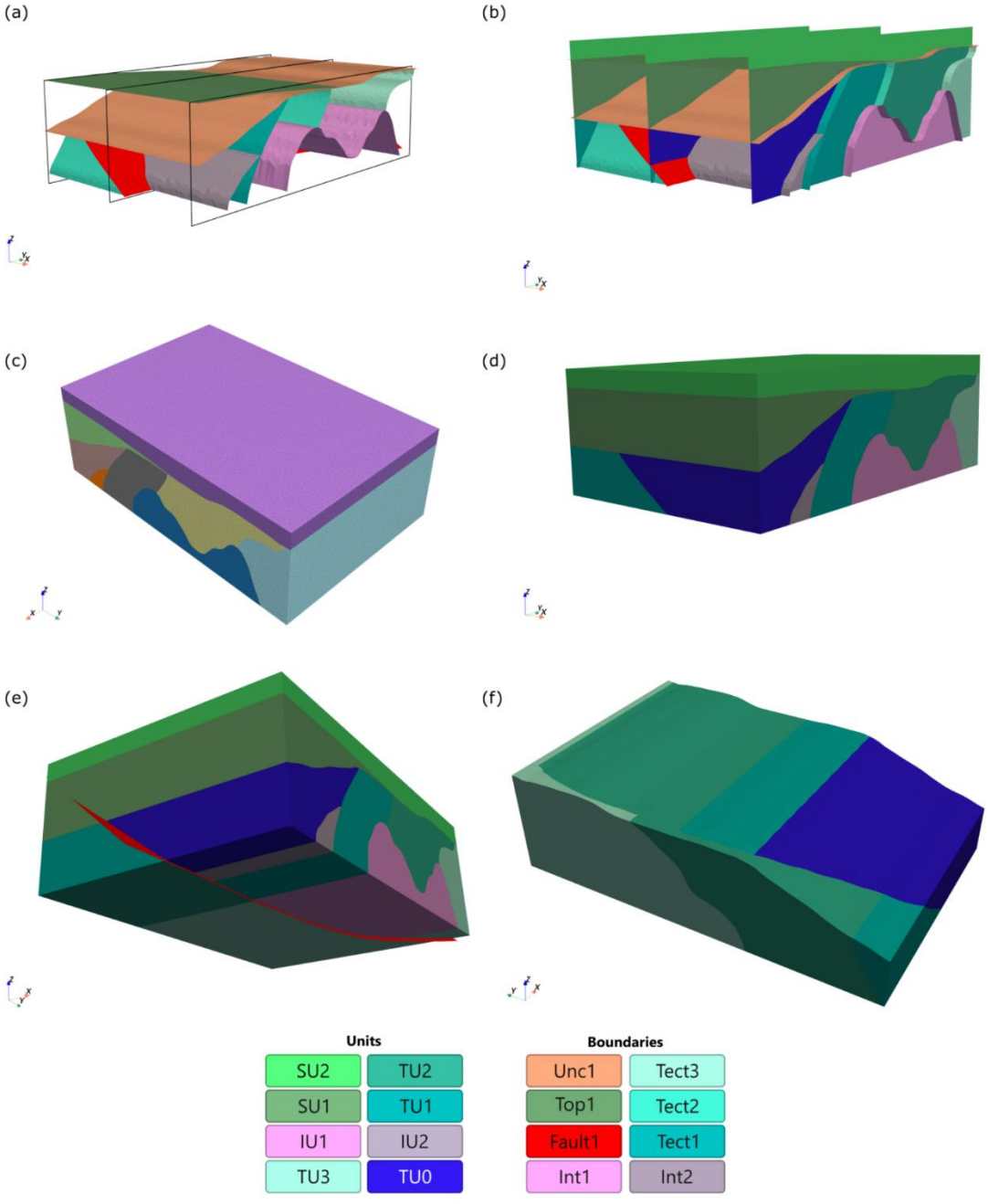


Figure 12: Overview of the synthetic 3D case study. (a) Geological surfaces used to construct the model, together with the traces of the three representative cross-sections shown in Fig. 11. (b) Geological surfaces and cross-sections after 2D PSC polygonization, showing the resulting section partitions. (c) Tetrahedral mesh generated in PyMeshIt. Colours in this panel correspond to the internal PyMeshIt colormap and therefore do not match the STM colour scheme used elsewhere in the model. (d–e) Different views of the tetrahedral model with 3D PSC material assignment exported to PZero; in (e), Fault1 is highlighted to improve visualization of its geometry and displacement relationships. (f) View of the Basement domain only, with the overlying stratigraphic cover removed to expose the internal tectonic and intrusive architecture.

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5.2.2 Llyn Padarn model

The Llyn Padarn case is based on a modified and simplified geological dataset inspired by the British Geological Survey 1:25,000 Llyn Padarn Classical Areas map (British Geological Survey, 1988). The model is not intended to reproduce the geology of the area in detail, but retains a strongly folded stratigraphic architecture, variable layer thicknesses, and fault offsets that make it suitable for testing the STM–PSC workflow under geometrically complex conditions. Topography is represented using the Copernicus EU-DEM v1.1 dataset (European Environment Agency, 2016). The model includes the Fachwen, Llanberis Slates, Bronllwyd Grit, Marchlyn and Nant Ffrancon formations, together with an additional informal unit (Above_NantF) introduced to complete the modelled succession (Fig. 13). For the purposes of the STM, these are represented as stratigraphic units (SUs).

Despite the geometrical complexity of the folded succession, its STM topology is comparatively simple. Stratigraphic boundaries are defined as conformable with respect to the adjacent units and the corresponding locked top–base relationships provide strong directional constraints. The automatic SL calculation therefore resolves the structural ordering of the succession without significant ambiguity (Fig. 13c).

A representative cross-section was constructed through the model and intersected with the topographic profile derived from the DEM (Fig. 13a-b).

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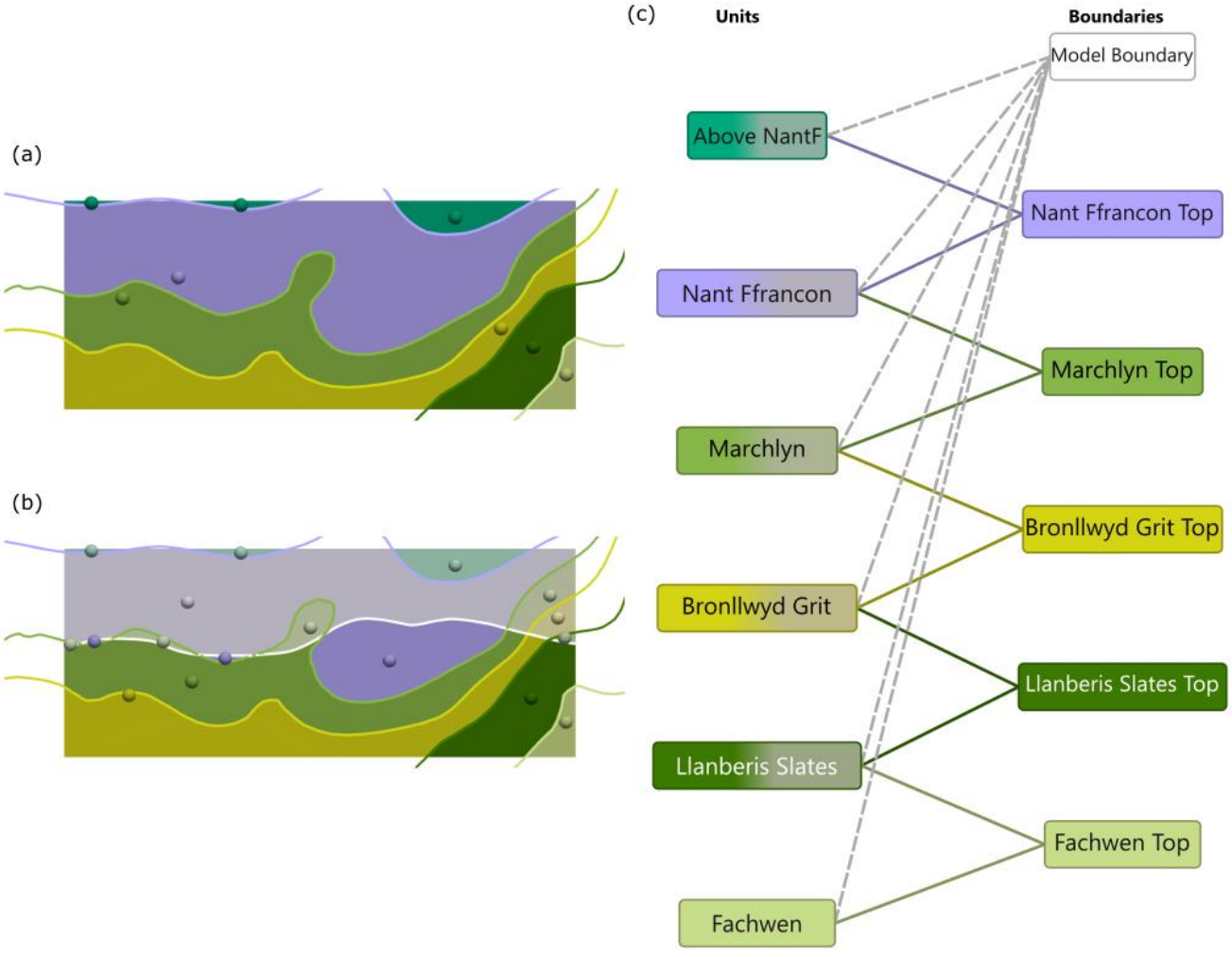


Figure 13: Llyn Padarn cross-section and STM representation. (a) Polygonized cross-section using the Model Boundary, to delimit the geological partition. (b) The same cross-section after applying the topographic profile to distinguish subsurface and eroded portions. (c) Exported STM graph corresponding to the model. Unit boxes use a dual colour representation, with the left side showing the original STM colour used for subsurface portions and the right side the corresponding desaturated colour used for eroded occurrences.

The tetrahedral model was then constructed in three different configurations. In the first (Fig. 14d), the DEM was not included and material attribution was performed directly using the 3D PSC. In the second (Fig, 14e), the DEM-based distinction between subsurface and eroded portions was transferred to PyMeshIt through the section-derived seeds, which currently provide the required metadata for this classification. In this configuration, eroded occurrences retain their individual geological identities. A third model was generated from the same section-derived information (Fig. 14f), but the eroded occurrences were assigned to a single virtual material during seed import.

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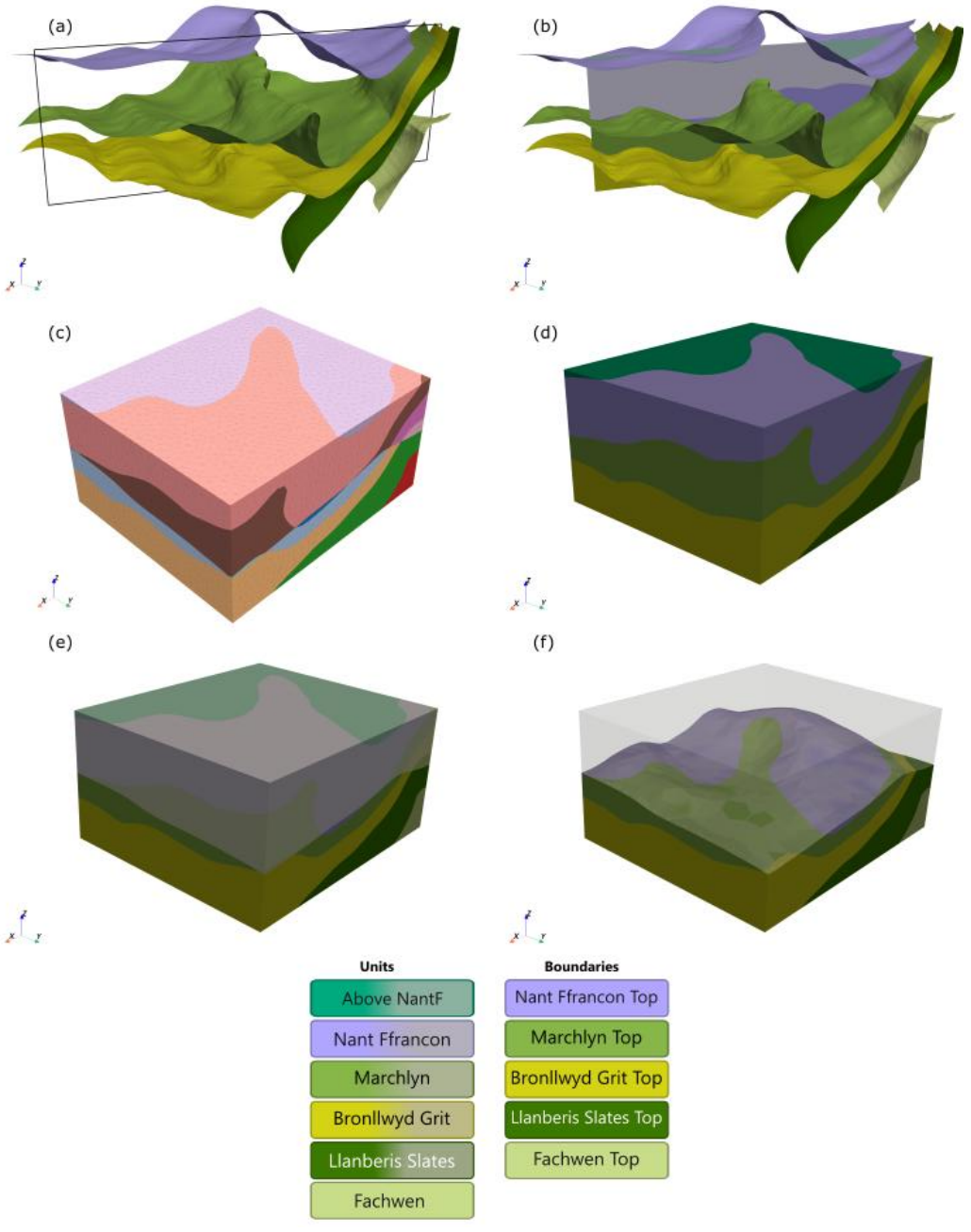


Figure 14: Overview of the Llyn Padarn 3D case study. (a) Geological surfaces used to construct the model, together with the trace of the representative cross-section. (b) Geological surfaces and cross-section after 2D PSC polygonization, showing the resulting section partition. (c) Tetrahedral mesh generated in PyMeshIt, including the DEM. Colours in this panel correspond to the internal PyMeshIt colormap and therefore do not match the STM colour scheme used elsewhere in the model. (d) Tetrahedral model exported to PZero without the DEM-based subdivision into subsurface and eroded portions. (e) DEM-constrained model in PZero, with eroded occurrences retaining their individual geological identities. (f) Alternative DEM-constrained representation in which the eroded occurrences are assigned to a common eroded material and displayed transparently to improve visualization of the topographic surface.

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The DEM-constrained configurations also expose a limitation of relying on seeds derived from a single cross-section. Because of the strongly folded geometry, some units occur as small disconnected eroded volumes that are not intersected by the selected section. In this example, three such volumes receive no section-derived seed and consequently remain unassigned during tetrahedral material attribution (Fig. 15). These occurrences can be resolved either by introducing additional cross-sections that intersect the missing volumes or by manually adding the corresponding material seeds in PyMeshIt.

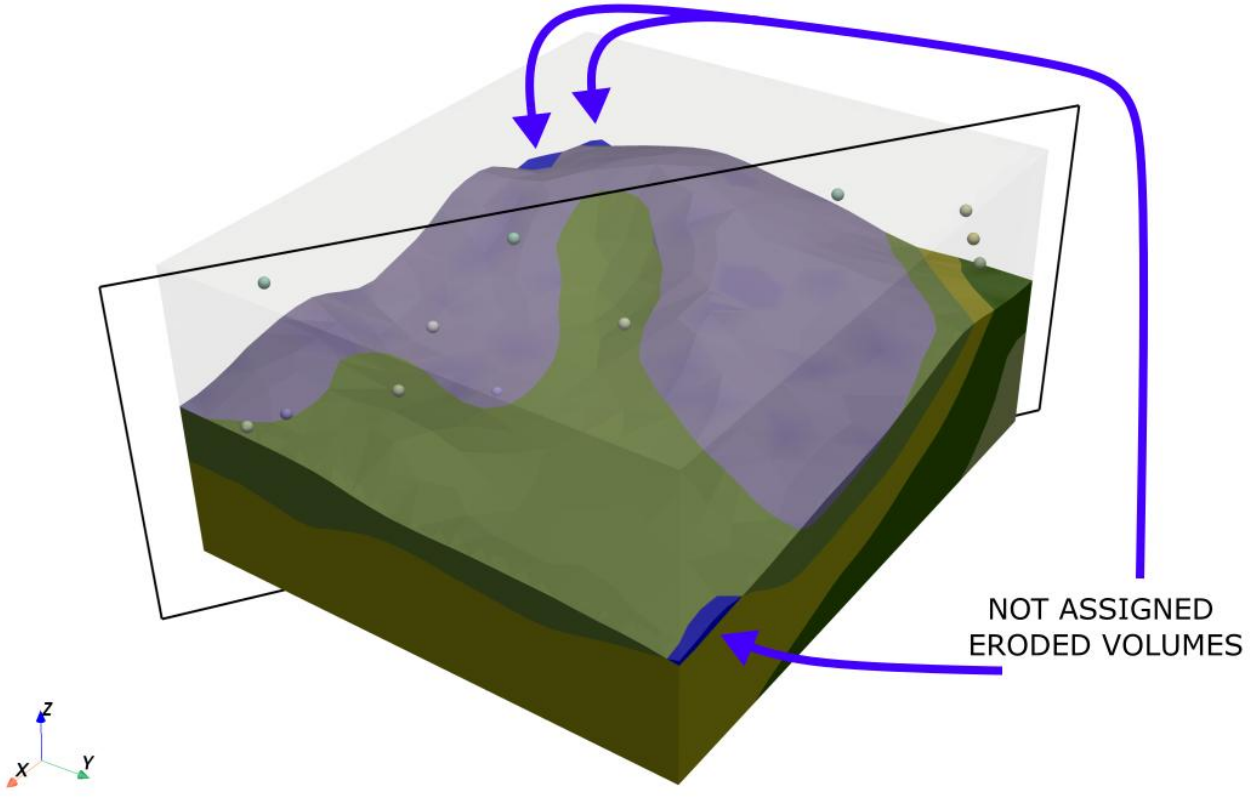


Figure 15: DEM-constrained Llyn Padarn tetrahedral model with eroded occurrences assigned to a common eroded material. The representative cross-section is shown together with the section-derived XsVertex seeds used for material attribution. Three disconnected eroded volumes that are not intersected by the section and therefore receive no corresponding seed remain unassigned and are highlighted in blue.

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5.2.3 Utah FORGE model

The second real 3D case revisits the Utah FORGE model previously tested with PyMeshIt by Hussain et al. (2026), based on the three-dimensional geological model released for the FORGE site near Milford, Utah The FORGE reservoir is hosted predominantly within fractured crystalline rocks, for which discrete fracture representations are commonly used in numerical modelling (Nadimi et al., 2020). In the present test, the model is therefore simplified into two units, the granitoid basement and the sedimentary cover, separated by an unconformity (Fig. 16).

Five finite fractures intersecting one of the well trajectories within the granitoid were retained to test their effect on volumetric partitioning (Fig. 16c). Although these fractures are represented explicitly as structural features, they remain entirely intraformational and do not act as boundaries between STM units. In this configuration, they do not separate connected volumetric regions and therefore do not contribute to the local PSC topological signatures. The well trajectory is likewise excluded from the PSC partition.

The two geological units have identical topological signatures, being both related to the unconformity and the model boundary through unconformable relationships. Their material attribution is consequently ambiguous from topology alone and requires user selection.

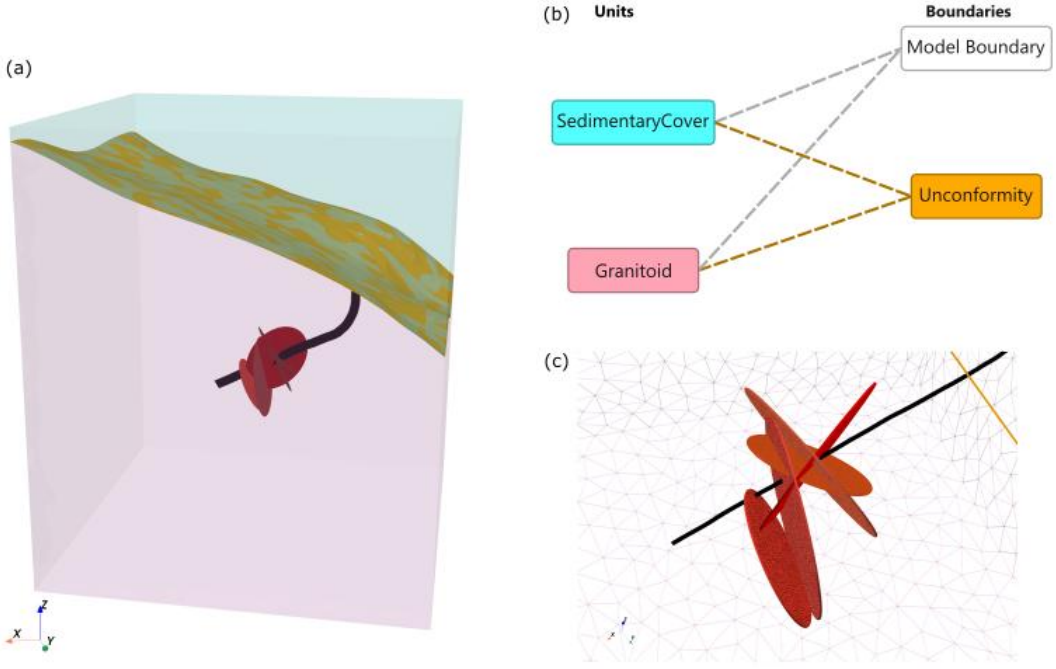


Figure 16: Overview of the Utah FORGE 3D case study. (a) Tetrahedral model with the geological units displayed transparently to improve visualization of the basal unconformity, the well trajectory, and the selected finite fractures. (b) Exported STM graph representing the simplified geological topology adopted for the model. (c) Detail of the finite fractures along the well within the tetrahedral mesh in granitoid unit.

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6 Discussion

The STM implementation presented in this work provides a framework for explicitly linking geology, topology, and geometrical partitioning with PSC within the PZero modelling environment through an ontology. The proposed approach addresses how geological relationships can be formalized before and during model construction, how they can constrain automatic attribution in 2D and 3D, and how uncertainty can be retained when the available information does not support a unique interpretation. The following sections discuss these methodological aspects together with their practical consequences in the implemented STM–PSC workflows.

6.1 Structural Levels and the formalization of structural ordering

The automatic calculation of SL provides one way of exploiting the relationships encoded in the STM. The benchmark cases show that the possibility of obtaining a unique structural ordering depends on the constraints encoded in these relationships, rather than on geometrical complexity alone.

The examples illustrate different degrees of constraint. In Cross-section 1, the encoded relationships allow the structural ordering to be resolved, whereas TU1 and SU7 in Cross-section 2 retain multiple admissible positions. Cross-section 3 further demonstrates that even complete topological relationships may admit alternative structural orderings when two units are topologically equivalent. In these cases, preserving alternative globally compatible configurations is preferable to introducing an arbitrary numerical ordering. The sequential resolution implemented in the STM Builder reduces the alternatives after each user decision while maintaining compatibility with the complete configuration.

The resulting user interaction therefore remains an interpretative step rather than a correction of an automatic failure.

Intrusive units constitute a particular case because their structural position is controlled primarily by intrusive contacts. The synthetic 3D model nevertheless highlights a current asymmetry: the relative-age information carried by an intrusive contact can constrain the intrusive unit without being fully propagated back to the host unit (Fig. 11d). In particular, TU0 requires a manual SL correction to respect its relative ordering with IU2, despite the initially calculated position satisfying the implemented topological constraints. This illustrates how a formally admissible configuration may remain inconsistent with geological relationships that have not yet been fully incorporated into the solver.

At present, the direct practical role of SL within PZero remains more limited than its conceptual role within STM. Boundary SL values are associated with the *Level* information used by the LoopStructural-based interpolation implemented in PZero, whereas unit SL values currently contribute mainly to surface extraction. This does not reduce their theoretical relevance: a scalar ordering of both boundaries and units provides a basis for introducing stronger geological constraints in future implicit-modelling workflows. A possible development would be to incorporate the unit–boundary relationships encoded in the STM as additional constraints in implicit modelling, alongside structural observations. A related extension would be to represent geological domains as explicit elements of the STM graph, rather than only as hierarchical unit groupings, potentially

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supporting the definition of domain-scale relationships. Both developments remain outside the scope of the present implementation.

795

6.2 PSC attribution

The benchmark cases demonstrate that the reliability of PSC attribution depends not only on the geometrical partition, but also on the completeness and discriminatory value of the geological boundary information available for each region. As illustrated by the synthetic 3D benchmark, different occurrences of the same geological unit may expose different subsets of its global
800 STM signature. The Max missing parameter controls the tolerated incompleteness by limiting the number of expected boundaries absent from an otherwise admissible match. Its appropriate value therefore depends on the geometry and extent of the local observation. Increasing this tolerance can recover otherwise unassigned regions, but may also introduce additional admissible candidates. The parameter should therefore be regarded as a tolerance for incomplete topological observations rather than a measure of geological confidence.
805 The synthetic 3D benchmark further illustrates how repeat validation can reject assignments that appear admissible when individual regions are considered in isolation. This provides an additional consistency check, although it does not amount to a simultaneous optimisation of all possible regional assignments. The Cross-section 3 and Utah FORGE benchmarks demonstrate a different limitation: distinct geological units may remain topologically indistinguishable even when their observed signatures are complete. In this case, even exact matches may not define a unique geological identity, and adjacent
810 ambiguous regions may admit several compatible joint assignments. The current implementation retains the AMBIGUOUS status and may provide provisional deterministic labels, without resolving the underlying geological ambiguity. Unlike the SL solver, which evaluates globally compatible structural-level configurations, the PSC does not currently enumerate all globally compatible combinations of ambiguous regional assignments. The current implementation therefore adopts a conservative strategy: unsupported assignments remain AMBIGUOUS or UNASSIGNED, preserving geological uncertainty for expert
815 interpretation rather than resolving it arbitrarily.

6.3 Structural features and partition boundaries

A relevant consequence of the STM–PSC approach is that geological discontinuities and effective partition boundaries are not necessarily equivalent. A structural feature may be geologically relevant without subdividing a unit into distinct model regions.
820 In 2D, this is illustrated the lower segment of F2 in Cross-section 2, which terminates within TU1 and is retained as an internal structural feature without being included in the sealed polygonization network. In 3D, surfaces that do not interrupt tetrahedral connectivity may similarly be retained as internal discontinuities without contributing to the PSC signature.

The Utah FORGE case illustrates this distinction for finite intraformational fractures, which remain represented in the tetrahedral model for numerical modelling without generating artificial geological subdivisions. Conversely, where
825 deformation is distributed over a finite volume, SDs may provide a suitable representation for assigning distinct physical or numerical properties to structurally affected regions in subsequent simulations. A limitation arises when discrete

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discontinuities intersect and geometrically isolate a closed volume: if its local signature does not correspond to any STM unit, the region remains unassigned. Geometrical closure is therefore not considered sufficient evidence for geological identity.

This distinction avoids forcing every mapped or modelled discontinuity to act as a unit boundary, which would otherwise generate partitions with limited geological significance.

6.4 Complementarity of 2D and 3D attribution

The 2D and 3D PSC procedures are independent attribution workflows, while section-derived seeds provide an optional connection between them. Direct 3D PSC exploits the topology of the reconstructed volumetric partition and can attribute regions independently of their intersection with a selected cross-section, whereas section-derived seeds transfer interpretations already inspected and controlled in cross-section.

The synthetic 3D case shows that both approaches can produce the same final material attribution, while also demonstrating that the information content of individual sections depends on their position and orientation. Section-derived attribution is therefore inherently local, but this selectivity is also one of its strengths: it allows geological relationships to be inspected and edited explicitly before transfer to the volumetric model.

Direct 3D PSC and section-derived seeds should consequently be considered complementary rather than alternative strategies, combining global topological attribution with local expert control.

6.5 Topographic information and DEM-constrained modelling

The Llyn Padarn case introduces an additional geometrical classification based on the present-day topographic surface. The distinction between subsurface and eroded occurrences does not modify STM signatures or PSC matching criteria, but is applied to already attributed geological units.

In the current implementation, this information is transferred to PyMeshIt through section-derived seeds, allowing eroded occurrences either be represented by distinct virtual materials derived from their original geological assignments or to share a single virtual material. Complex geometries, however, may generate disconnected eroded volumes not intersected by the selected section and therefore lacking a corresponding seed.

Additional sections or manually introduced seeds provide practical solutions, while a future direct DEM-based classification of reconstructed 3D PSC regions could provide more complete volumetric coverage.

This should not replace the section-based approach, which remains valuable for visualization and expert-controlled attribution, but would reduce the dependence of topographic classification on section sampling.

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7 Conclusion

This work introduces the implementation of the Structural Topology Model (STM) in PZero and its integration with 2D and 3D Piecewise Structural Complex (PSC) procedures for geological partitioning and material attribution. The approach formalizes geological units, boundaries, Structural Level (SL), conformability, hierarchy, and topological signatures independently from their final geometrical representation, allowing this information to be used directly during model construction and attribution in both cross-sections and tetrahedral models.

The synthetic and real examples show that this formulation is particularly useful when geological information is incomplete or non-unique. Topology-constrained SL calculation can resolve structural ordering where sufficient relationships are available, while retaining alternative admissible positions when they are not. Partial signatures can be associated with their global units within a controlled tolerance, structural repetitions are distinguished from incompatible duplicates through unit-specific conformability, and equivalent signatures remain explicitly ambiguous when topology alone cannot discriminate between alternative interpretations. Structural discontinuities can also remain represented without necessarily acting as unit boundaries, avoiding unnecessary subdivision of geological volumes. The resulting behaviour is deliberately conservative: when the encoded constraints are insufficient, PSC assignments retain an AMBIGUOUS or UNASSIGNED status rather than imposing an unsupported geological attribution.

The implementation also provides complementary links between 2D interpretation and 3D modelling. Direct 3D PSC uses the topological relationships of the reconstructed volumetric partition, whereas section-derived seeds allow expert-controlled 2D assignments to be transferred to PyMeshIt. Topographic information can further distinguish subsurface and eroded occurrences without modifying STM signatures.

Several developments could further extend the present framework, including a more complete propagation of cross-cutting age relationships, globally coupled resolution of PSC ambiguities, and direct DEM-based classification of 3D regions. Overall, the STM–PSC implementation demonstrates how geological topology can become an operational component of model construction rather than remaining implicit in the interpreter's conceptual model. By constraining automation without suppressing geological uncertainty, the framework provides a consistent link between geological reasoning, geometrical partitioning, and 2D–3D model attribution.

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Code and data availability

PZero, the geological modelling environment used in this study, is open-source and available at https://github.com/gecos-lab/PZero under the GNU Affero General Public License v3.0. Specifically, the tools described in this study are implemented starting from PZero 2.0. All the case studies are available at https://doi.org/10.5281/zenodo.23690665.

Author contributions

RM conceived the study, developed the PSC methodology and the underlying algorithms, constructed the synthetic geological models, performed the benchmark tests, analysed and validated the results, prepared the visualizations, and wrote the original draft. RM and WH jointly contributed to the implementation of the STM and PSC algorithms in PZero. WH also provided technical expertise on PyMeshIt, supported the integration of the PSC workflow with the meshing framework, and contributed to methodological discussions and validation. MC contributed to the review, refinement, and validation of the proposed methodology and its implementation, as well as to critical review and editing of the manuscript. AB supervised the research, contributed to the conceptual development of the underlying theoretical framework, and provided scientific guidance and critical review and editing of the manuscript. All authors discussed the results, reviewed the manuscript, and approved its final version.

Competing interests

The contact author has declared that none of the authors has any competing interests.

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OpenAI Codex, using the Sol 5.6 and Sol 6.1 models, was used to assist with code development, implementation, and debugging. All AI-assisted code was reviewed, tested, and validated by the authors, who retain full responsibility for the software and the results presented.

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