3D Geomodelling of Alpine structures with PZero

Riccardo Monti[1], Andrea Bistacchi[1], Gabriele Benedetti[1], and Waqas Hussain[1]

[1] *GECOS Lab, Dipartimento di Scienze dell'Ambiente e della Terra, Università degli Studi di Milano-Bicocca, 20126, Italy*.

September 2024

Abstract

Three-dimensional geological modelling is a rapidly growing field of interest and application, both in research and industry, leading to the emergence of open-source software to make this technology more accessible. Here we present PZero, an open-source software written in Python, created and developed by GECOS-LAB (github.com/gecos-lab) and supported by the GeoSciences IR project (geosciences-ir.it). PZero is a 3D geological modelling software with a user-friendly graphical interface (built with Qt) designed for the (structural) geologist, allowing both explicit and implicit interpolation (using LoopStructural) of geological structures from different input datasets, including field geological and structural surveys, Digital Outcrop Models, but also subsurface data such as wells and seismics. One important development branch of PZero is focused on modelling strategies and interpolation algorithms for 3D modelling of complex ductile structures, such as refolded isoclinal folds and shear zones. For this task we have selected a case study from the Penninic Domain of the Central Alps, characterized by continental and oceanic units that were deeply involved in subduction- and collision-related tectonics, then exhumed and crosscut by late-stage brittle faults, resulting in very challenging natural laboratory, where the latest modelling strategies can be tested in depth.

Introduction

In the last decade, three-dimensional geological modelling has become an increasingly fundamental tool in more widespread fields of geology, such as structural geology, engineering geology, ore and oil industry, and energy transition (WELLMANN & CAUMON, 2018). Owing to the increasing computational power and growing demand for 3D models from small companies, public agencies (e.g. geological surveys) and research groups, the necessity to represent complex geological features has led to the emergence of open-source algorithms and software based on different statistical methods that aim at making 3D modelling more accessible, also increase the reproducibility of the models leveraging on the implicit approach (e.g. DE LA VARGA, SCHAAF & WELLMANN, 2019; GROSE ET AL., 2021; HILLIER ET AL., 2023; MALARD ET AL., 2023).

In this work, we present new developments of PZero, a Python open-source 3D geological modelling software born in 2020, originally funded by Pro Iter Tunnelling & Geotechnical Department, and currently in development by GECOS-LAB and supported by the GeoSciences IR project led by ISPRA – Servizio Geologico d'Italia. PZero features a user-friendly Qt graphical interface (Fig. 1) with different windows (e.g. 3D View, Map View, etc.). It can accept a variety of different inputs formats, such as SHP files, GOCAD ASCII, SEGY, DEM and imagery as GeoTIFF, point clouds, and wells, converting all of them into

VTK objects. Additionally, it allows exporting these objects in the same formats listed above, plus CAD formats with CSV metadata, to ensure interoperability with engineering software.

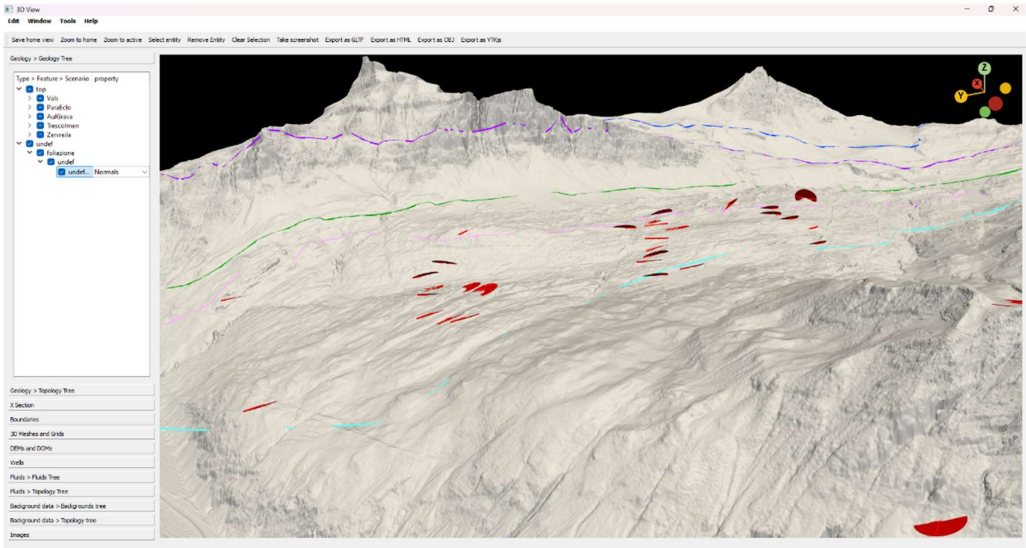

Figure 1, 3D View in PZero showing the Digital Elevation Model (DEM) and units' top and dips projected on it.

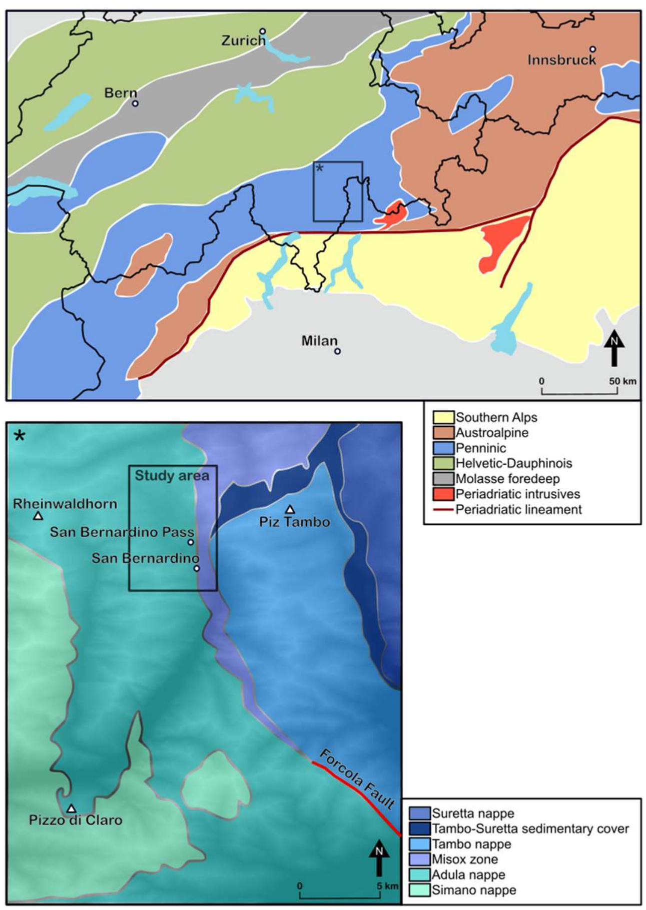

Figure 2, Tectonic sketch map of Western and Central Alps and regional setting of the study area (modified after Malusà et al., 2015, Cavargna-Sani et al., 2014).

Thanks to various Python libraries, PZero implements different data management and analysis tools, DOM analysis (Benedetti et al., 2023), explicit surfaces interpolators and – thanks to the LoopStructural library – three different algorithms for time-aware implicit interpolation (Grose, Ailleres, Laurent & Jessell, 2021).
In this contribution we present a case study in the area of the San Bernardino Pass in Switzerland (Fig. 2), an Alpine pass at 2065 m a.s.l. in the Moesa region of Canton Grisons. In the area of the pass, the contact between the Adula nappe and the Misox Zone – a km-thick shear zone that separates the Adula from the overlying Tambo nappe – is exposed (Cavargna-Sani, Epard & Steck, 2014; Pleuger et al., 2003). These nappes belong to the eastern flank of the Lepontine Dome, an important structure of the Pennine domain constituted by oceanic and continental nappes derived from the distal margin of the European plate (Dal Piaz, Bistacchi & Massironi, 2003; Schmid et al., 2004). The units of the Lepontine Dome show a high-pressure metamorphism in blueschist and eclogitic facies, generally obliterated by syn-collisional metamorphism of the Barrovian type in greenschist to amphibolite facies (Malusà et al., 2015; Nagel, 2008). The Adula nappe and the Adula-Cima Lunga complex are well-known geological units because of the presence of eclogites and peridotites of high and ultra-high pressure with both Varisican and Alpine ages (Sandmann et al., 2014). In the study area, the Adula nappe is represented by paragneisses and the Zervreila orthogneiss derived from a Permian intrusion, together constituting large scale isoclinal folds refolded by successive deformative events, together with the nappes stacking recorded in a pervasive top-to-NW foliation developed at 35 Ma (Zapport phase)

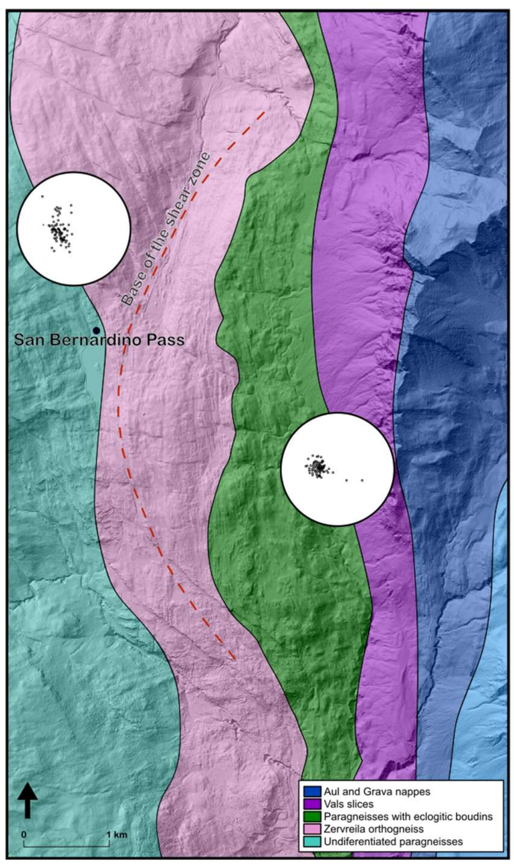

Figure 3, Simplify geological map of the study area (see Fig.2) superposed on the hillshade, where the folded area is recognizable under the base of the shear zone (on the left). The mylonitic orthogneisses outcrop just above the base of the shear zone.

(Marquer, Challandes & Baudin, 1996; Pleuger et al., 2003). The main isoclinal folds show E-W hinge lines with horizontal axial surfaces, in turn folded by gentle folds with E-W and E-dipping hinge lines and vertical axial surfaces. At the top of the nappe, a shear zone cuts the top of the Zervreila orthogneiss with the development of mylonites and ultramylonites, in turn overlain by paragneisses of the Adula Nappe with eclogitic boudins. In this shear zone (Fig.3), together with a strongly rectilinear SE-dipping and top-to-NW foliation, a quite pervasive top-to-E foliation – related to the exhumation of the Lepontine dome and consistent with the more southerly Forcola normal fault (Tagliaferri et al., 2023) – is present. This shear zone is linked with the Misox zone consisting of high-pressure-low-temperature metamorphic slices and nappes with sedimentary and MORB-derived protoliths, such as the Vals slices and the Aul and Grava nappes (Cavargna-Sani, Epard & Steck, 2014; Wiederkehr et al., 2011).

Methods

In order to produce a 3D model of the area of the San Bernardino Pass, we started from original field data and from and available geological maps (Cavargna-Sani, Epard & Steck, 2014; Pleuger et al., 2003). In order to model metamorphic nappes, it is essential to model both qualitatively and quantitatively the geometry of the contacts and their spatial position, and how structural data can be used as constraints. For instance the geometry of nappe boundaries can be constrained from the foliation near the boundaries (Fig.4).

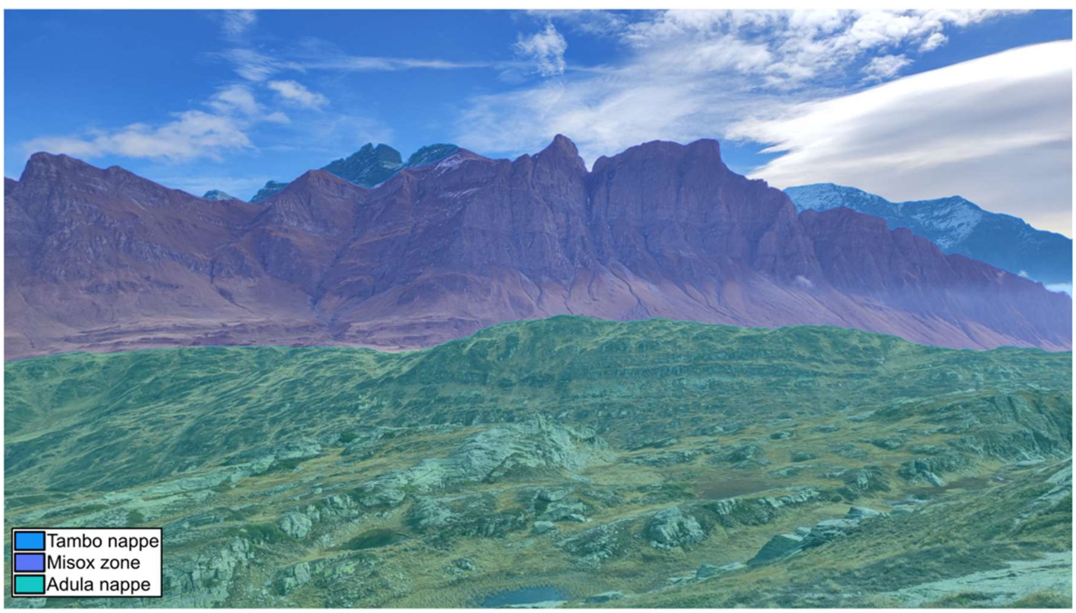

Figure 4, View of the San Bernardino Pass area and the outcropping nappes (LOOK E).

Our input data consist of a simplified geological map, created in QGis, imported in PZero and projected on the DEM (available on the SwissTopo geoportal; www.swisstopo.admin.ch) together with structural data. The distribution of input data over a rugged mountain topography allows interpreting all these data as a truly 3D input dataset.

Even if the LoopStructural library allows strong structural constraints (e.g. folds axial planes, folding wavelength, fault interaction ellipsoids, and fault intersections) to create folded frames (Grose, Ailleres, Laurent & Jessell, 2021; Grose et al., 2017, 2018; Laurent et al., 2016) and faulted frames (Grose, Ailleres, Laurent, Caumon et al., 2021), the time-aware legend implemented in PZero is not yet compatible with these tools, making the intervention of the structural geologist necessary in drawing geological cross sections to increase the number of constraints. According to the main structures, four NW-SE cross sections were drawn perpendicular to folds axial surfaces -in the western area, below the shear zone- to better constrain the refolded isoclinal folds and five E-W cross sections -in the eastern area and inside the shear zone- parallel to the dip direction of the mylonitic foliation, both with an inter-distance of 1 km (Fig.5).

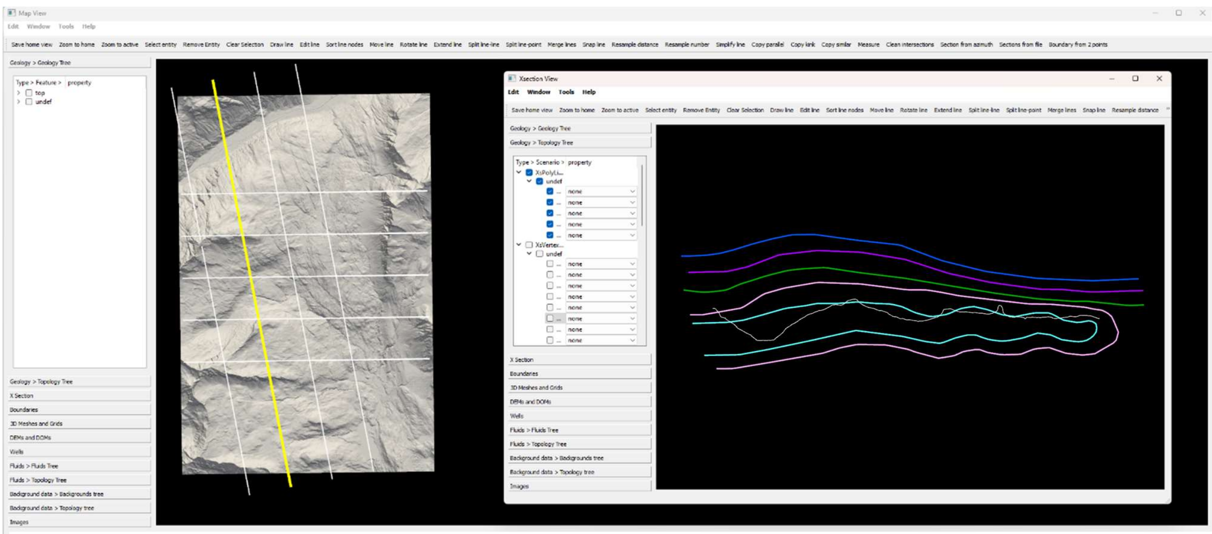

Figure 5, on the left Map View and main cross-sections; on the right the details of the selected cross-section (in yellow in the Map View) in the Xsection View with its interpretation and DEM intersection (in white).

Using a buffer of half the distance between two cross sections, dips were projected on them and their intersections with the top of the units and with the DEM were also plotted as constraints. Thanks to these projected objects it was possible to carry out a traditional, but quantitatively constrained, interpretation of the cross sections. Afterwards, other cross sections were created between the existing ones and near to the boundaries of the study area. To interpret these cross sections, the closest interpretated ones were projected on them and corrected using intersections constraints as described before. Resampling with 100 m steps was applied to all lines representing the tops of the units to increase the number of points to be used as input during interpolation.

Subsequently, in order to interpolate all field data and lines from cross-sections and to generate surfaces in a single computational process, we used the implicit approach. A bounding box was defined in the study area with a default number of cells equal to 62500 (50*50*25 as defined in LoopStructural) and a grid distance of about 155 m due to dimension of the box (Fig.6)

The implicit surfaces interpolator in LoopStructural is designed to find a function that represents the distance from a reference geological horizon by leveraging a weighted combination of basis functions:

$$f(x, y, z) = \sum_{i=0}^{N} v_i \varphi_i(X)$$

where N is the number of basis functions, v are the weights and φ are the basis functions (GROSE, AILLERES, LAURENT, CAUMON ET AL., 2021). Other observations used as constraints are the interface between geological units, the magnitude of the gradient norm and the orthogonal vector of the scalar field.

For this model, we used the Piecewise Linear Interpolation (PLI), one of the approaches for discrete interpolation in LoopStructural. It uses a linear function -called linear tetrahedron- that interpolates the property within the tetrahedron where it is applied (GROSE, AILLERES, LAURENT, CAUMON ET AL., 2021; *Implicit Interpolators — LoopStructural 1.6.0 documentation*, s. d.):

$$\phi(x, y, z) = a + bx + cy + dz$$

And for each node:

$$\phi_0 = a + bx_0 + cy_0 + dz_0,$$
$$\phi_1 = a + bx_1 + cy_1 + dz_1,$$
$$\phi_2 = a + bx_2 + cy_2 + dz_2,$$
$$\phi_3 = a + bx_3 + cy_3 + dz_3$$

The geological observations can be incorporated into the PLI by linear equations passing through the vertices of tetrahedrons. A constant gradient regularization(CAUMON ET AL., 2013; FRANK, TERTOIS & MALLET, 2007) is applied to minimize the gradient between neighboring tetrahedra:

$$\nabla\phi_{T_1} - \nabla\phi_{T_2} = 0$$

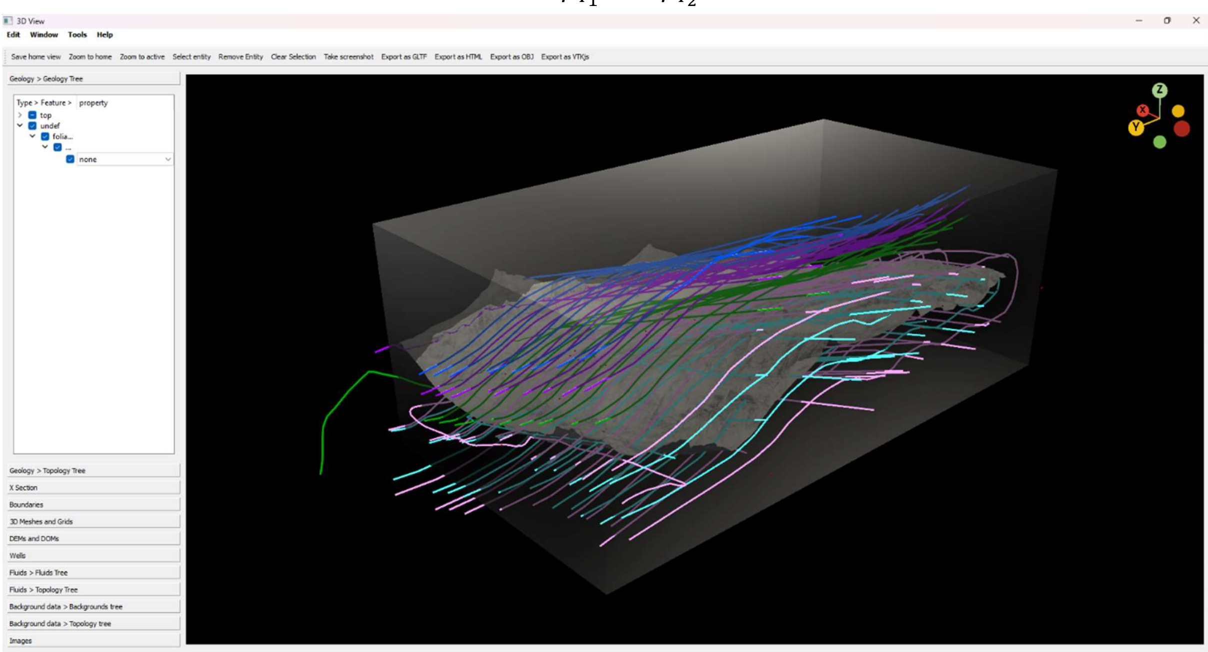

Figure 6, Bounding box used to create the scalar field interpolating the lines from the cross-section.

Results and discussion

The model we present in this work is an important step for the development of PZero. Despite it is still impossible in PZero to model faults with implicit methods (that would be useful to represent the base of our shear zone), we were able to create a coherent model of the transition between the folded area and the shear zone - where the foliation is rectilinear.

This limitation with faults creates difficulties in calculating the scalar field over the whole study area, since it is not possible to create discontinuities separating domains with different structures in the same bounding box. To overcome this problem, we first tried to interpolate the top surfaces of the units in the same bounding box – to preserve the same extent and

resolution – but modelling the two subareas separated by the base of the shear zone in two different computational processes, resulting in two scalar fields (Fig.7). In this way we easily interpolated the correct structures but encountered problems with overlap and intersection between the surfaces generated in the two processes – in particular, between the Zervreila orthogneiss and the overlying paragneisses with eclogitic boudins.
A second attempt was to increase the constraints by increasing the number of points within the sections in order to keep the geometries correct and at the same time generate surfaces that did not intersect each other.
In this case we observed as artifact an attempt to bend the surfaces within the shear zone below the refolded zone, creating a large-scale recumbent fold with a polydeformed core -folded area below the shear zone- and a slightly deformed outer part -inside the shear zone (Fig.8). To resolve this condition – but this is not a solution that we recommend for routine use – the fact that the hinge area of the artefact is outside the bounding box was exploited allowing the erroneously generated lower flank surfaces below the folded structures to be easily removed from the model. In this way it was possible to create a representative and consistent model of the area respecting the geometries of the folded isoclinal folds - where two folding events can be observed- and the overlying shear zone.
Despite the geologist intervention needed and the simplification of the complex folds interest the undifferentiated paragneisses and the Zervreila orthogneiss, we consider this model a valid result to represent the area of the San Bernardino Pass and its main structures. The first attempt should not be ruled out a priori, however, because subdivision into regions - using one or more boundary boxes - is a fundamental technique for 3D modelling of large areas (ARIENTI ET AL., 2024), but it is necessary to implement an algorithm in PZero that prevents intersections between different portions of the model.

Conclusion

This work shows that, even with technical limitations, it is possible to obtain consistent and detailed geological models using PZero. Geologist intervention remains critical for drawing cross sections and model refinements, particularly in the presence of complex geological structures. This study highlights the importance of continuing to develop more advanced modelling tools that can reduce the need for manual intervention, improving model automation and accuracy. In the future, PZero could benefit from the integration of fault and folds constraints algorithms to increase its ability to represent complex geological structures. Furthermore, the approach used in this work could be applied to other geological areas -such as from the Penninic Domain of the Central and Western Alps - with similar characteristics, contributing to a more detailed understanding of tectonic dynamics in different regions. With further development, PZero has the potential to become a key tool for structural geologists, providing increasingly accurate and useful models for research and practical applications.

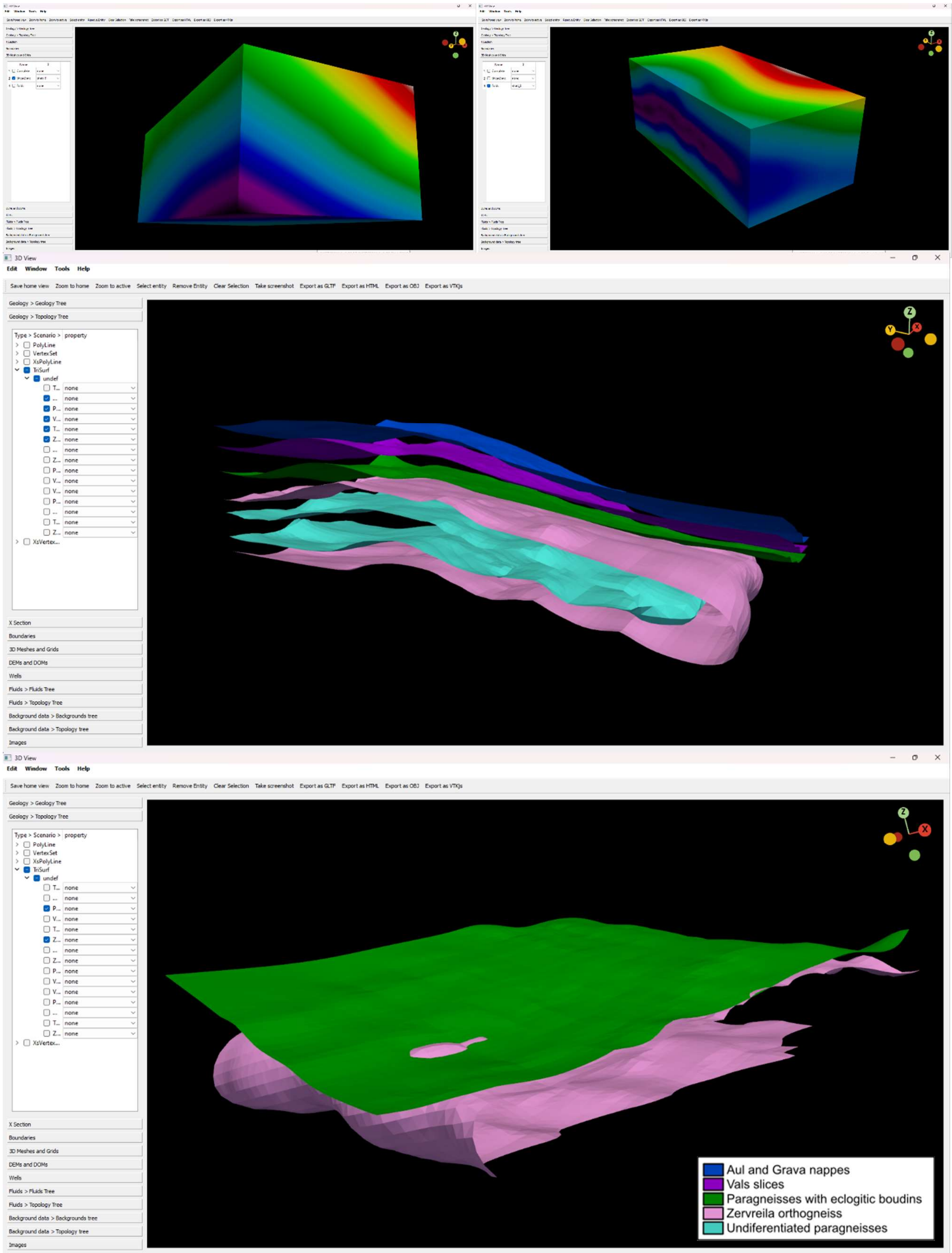

Figure 7, on top left: 3D mesh of the shear zone showing a regular E-dipping scalar field; on top right: 3D mesh of the folds showing folded structures in all the directions; in the center: surfaces extrapolated from the two scalar fields. On bottom: intersection and overlapping between the Zervreila orthogneiss and the paragneisses above.

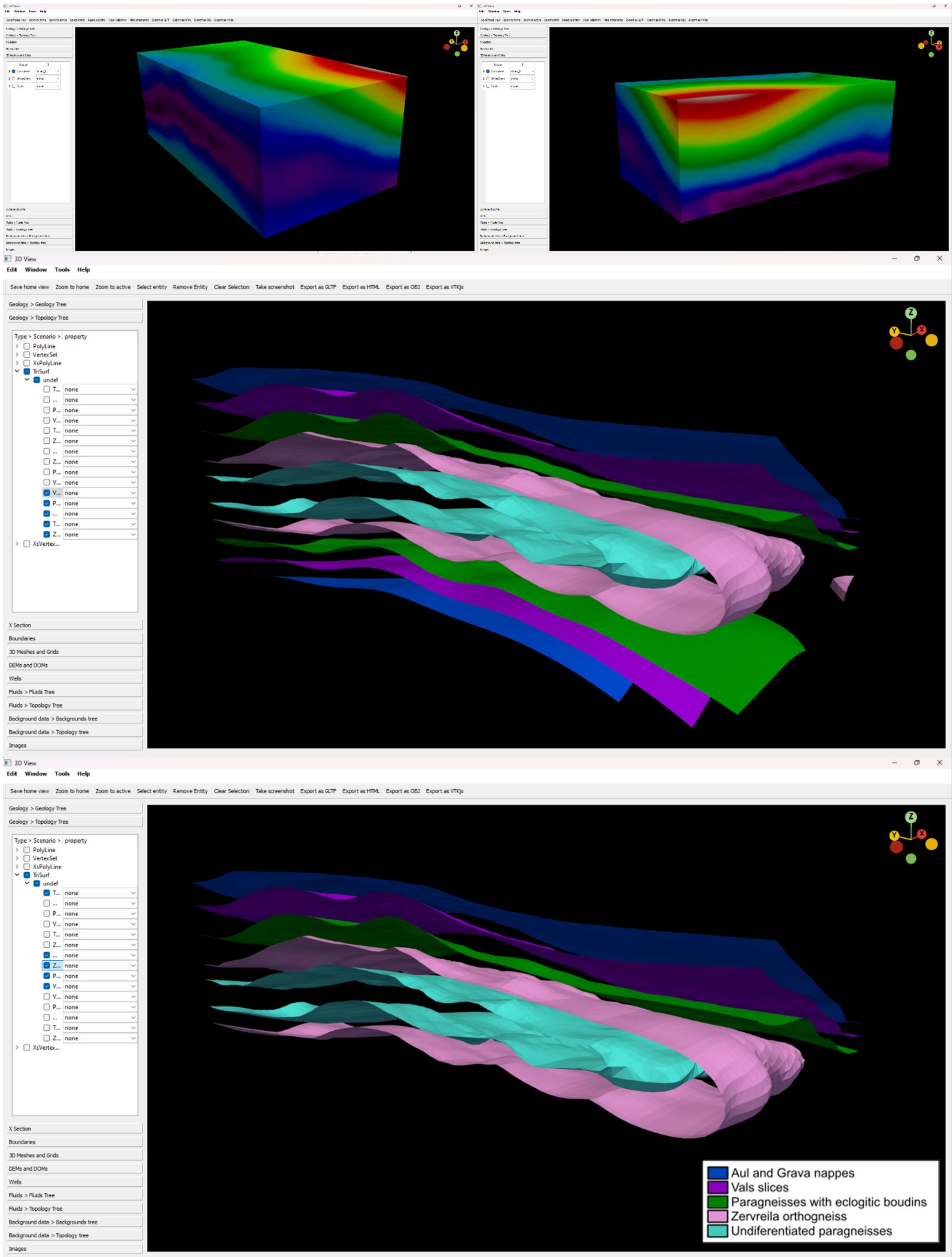

Figure 8, on top: 3D mesh of the complete dataset showing both the folds and the shear zone in the scalar field; in the center: surfaces extrapolated from the scalar field with a lower flank of the artefact fold. On bottom: surfaces with artefacts removed.

References

ARIENTI G, BISTACCHI A, CAUMON G, DAL PIAZ G, MONOPOLI B & BERTOLO D. (2024). Regional-scale 3D modelling in metamorphic belts: An implicit model-driven workflow applied in the Pennine Alps. *Journal of Structural Geology 180*:105045. https://doi.org/10.1016/j.jsg.2023.105045

BENEDETTI G, CASIRAGHI S, BISTACCHI A, ARIENTI G & BERTOLO D. (2023). Point cloud analysis and segmentation procedures in the PZero software. *EGU General Assembly Conference Abstracts*:EGU-9549. https://ui.adsabs.harvard.edu/abs/2023EGUGA..25.9549B/abstract

CAUMON G, PELLERIN J, LAURENT G, CHERPEAU N, LALLIER F, MERLAND R & BONNEAU F. (2013). Current bottlenecks in geomodeling workflows and ways forward. In: D Garner, D Thenin, & CV Deutsch (□ds.), *Closing the gap : advances in applied geomodeling for hydrocarbon reservoirs* (Vol. 20, p. 43-52). Canadian Society of Petroleum Geologists. https://hal.univ-lorraine.fr/hal-01963734

CAVARGNA-SANI M, EPARD J-L & STECK A. (2014). Structure, geometry and kinematics of the northern Adula nappe (Central Alps). *Swiss Journal of Geosciences 107*(2-3):135-156. https://doi.org/10.1007/s00015-014-0175-7

DAL PIAZ GV, BISTACCHI A & MASSIRONI M. (2003). Geological outline of the Alps. *Episodes Journal of International Geoscience 26*(3):175-180. https://doi.org/10.18814/epiiugs/2003/v26i3/004

DE LA VARGA M, SCHAAF A & WELLMANN F. (2019). GemPy 1.0: open-source stochastic geological modeling and inversion. *Geoscientific Model Development 12*(1):1-32. https://doi.org/10.5194/gmd-12-1-2019

FRANK T, TERTOIS A-L & MALLET J-L. (2007). 3D-reconstruction of complex geological interfaces from irregularly distributed and noisy point data. *Computers & Geosciences 33*(7):932-943. https://doi.org/10.1016/j.cageo.2006.11.014

GROSE L, AILLERES L, LAURENT G, CAUMON G, JESSELL M & ARMIT R. (2021). Modelling of faults in LoopStructural 1.0. *Geoscientific Model Development 14*(10):6197-6213. https://doi.org/10.5194/gmd-14-6197-2021

GROSE L, AILLERES L, LAURENT G & JESSELL M. (2021). LoopStructural 1.0: time-aware geological modelling. *Geoscientific Model Development 14*(6):3915-3937. https://doi.org/10.5194/gmd-14-3915-2021

GROSE L, LAURENT G, AILLÈRES L, ARMIT R, JESSELL M & CAUMON G. (2017). Structural data constraints for implicit modeling of folds. *Journal of Structural Geology 104*:80-92. https://doi.org/10.1016/j.jsg.2017.09.013

GROSE L, LAURENT G, AILLÈRES L, ARMIT R, JESSELL M & COUSIN-DECHENAUD T. (2018). Inversion of Structural Geology Data for Fold Geometry. *Journal of Geophysical Research: Solid Earth 123*(8):6318-6333. https://doi.org/10.1029/2017JB015177

HILLIER M, WELLMANN F, DE KEMP EA, BRODARIC B, SCHETSELAAR E & BÉDARD K. (2023). GeoINR 1.0: an implicit neural network approach to three-dimensional geological modelling. *Geoscientific Model Development 16*(23):6987-7012. https://doi.org/10.5194/gmd-16-6987-2023

Implicit Interpolators — LoopStructural 1.6.0 documentation. (s. d.). Consulté 5 juillet 2024, à l'adresse https://loop3d.org/LoopStructural/user_guide/interpolation_options.html

LAURENT G, AILLERES L, GROSE L, CAUMON G, JESSELL M & ARMIT R. (2016). Implicit modeling of folds and overprinting deformation. *Earth and Planetary Science Letters 456*:26-38. https://doi.org/10.1016/j.epsl.2016.09.040

MALARD A, DÖRFLIGER N, JEANNIN P-Y & LAUBE S. (2023). Contribution of the dynamic visualization of a 3D hydrogeological conceptual model to the participatory management of groundwater resources. *Comptes Rendus. Géoscience 355*(S1):231-244. https://doi.org/10.5802/crgeos.152

MALUSÀ MG, FACCENNA C, BALDWIN SL, FITZGERALD PG, ROSSETTI F, BALESTRIERI ML, DANIŠÍK M, ELLERO A, OTTRIA G & PIROMALLO C. (2015). Contrasting styles of (U)HP rock exhumation along the Cenozoic Adria-Europe plate boundary (Western Alps, Calabria, Corsica). *Geochemistry, Geophysics, Geosystems 16*(6):1786-1824. https://doi.org/10.1002/2015GC005767

MARQUER D, CHALLANDES N & BAUDIN T. (1996). Shear zone patterns and strain distribution at the scale of a Penninic nappe: the Suretta nappe (Eastern Swiss Alps). *Journal of Structural Geology 18*(6):753-764. https://doi.org/10.1016/S0191-8141(96)80009-5

NAGEL TJ. (2008). Tertiary subduction, collision and exhumation recorded in the Adula nappe, central Alps. *Geological Society, London, Special Publications 298*(1):365-392. https://doi.org/10.1144/SP298.17

PLEUGER J, HUNDENBORN R, KREMER K, BABINKA S, KURZ W, JANSEN E & FROITZHEIM N. (2003). *Structural evolution of Adula nappe, Misox zone, and Tambo nappe in the San Bernardino area: Constraints for the exhumation of the Adula eclogites*.

SANDMANN S, NAGEL TJ, HERWARTZ D, FONSECA ROC, KURZAWSKI RM, MÜNKER C & FROITZHEIM N. (2014). Lu–Hf garnet systematics of a polymetamorphic basement unit: new evidence for coherent exhumation of the Adula Nappe (Central Alps) from eclogite-facies conditions. *Contributions to Mineralogy and Petrology 168*(5):1075. https://doi.org/10.1007/s00410-014-1075-6

SCHMID SM, FÜGENSCHUH B, KISSLING E & SCHUSTER R. (2004). Tectonic map and overall architecture of the Alpine orogen. *Eclogae Geologicae Helvetiae 97*(1):93-117. https://doi.org/10.1007/s00015-004-1113-x

TAGLIAFERRI A, SCHENKER FL, ULIANOV A, MAINO M & SCHMALHOLZ SM. (2023). Implications of New Geological Mapping and U-Pb Zircon Dating for the Barrovian Tectono-Metamorphic Evolution of the Lepontine Dome (Central European Alps). *Geochemistry, Geophysics, Geosystems 24*(3):e2022GC010772. https://doi.org/10.1029/2022GC010772

WELLMANN F & CAUMON G. (2018). 3-D Structural geological models: Concepts, methods, and uncertainties. In: *Advances in Geophysics* (Vol. 59, p. 1-121). Elsevier. https://doi.org/10.1016/bs.agph.2018.09.001

WIEDERKEHR M, BOUSQUET R, ZIEMANN MA, BERGER A & SCHMID SM. (2011). 3-D assessment of peak-metamorphic conditions by Raman spectroscopy of carbonaceous material: an example from the margin of the Lepontine dome (Swiss Central Alps). *International Journal of Earth Sciences 100*(5):1029-1063. https://doi.org/10.1007/s00531-010-0622-2