

# Three-dimensional gravity anomaly inversion in the Pyrenees using compressional seismic velocity model as structural similarity constraints

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#### 6 SUMMARY

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We explore here the benefits of using constraints from seismic tomography in gravity 8 data inversion and how inverted density distributions can be improved by doing so. The 9 methodology is applied to a real field case in which we reconstruct the density struc-10 ture of the Pyrenees along a southwest-northeast transect going from the Ebro basin in 11 Spain to the Arzacq basin in France. We recover the distribution of densities by invert-12 ing gravity anomalies under constraints coming from seismic tomography. We initiate the 13 inversion from a prior density model obtained by scaling a pre-existing compressional 14 seismic velocity  $V_p$  model using a Nafe-Drake relationship : the  $V_p$  model resulting from 15 a full-waveform inversion of teleseismic data. Gravity data inversions enforce structural 16

similarities between  $V_p$  and density by minimizing the norm of the cross-gradient between the density and  $V_p$  models. We also compare models obtained from 2.5D and 3D inversions. Our results demonstrate that structural constraints allow us to better recover the density contrasts close to the surface and at depth, without degrading the gravity data misfit. The final density model provides valuable information on the geological structures and on the thermal state and composition of the western region of the Pyrenean lithosphere.

Key words: Gravity Modelling – Data inversion – Seismic correlation and constraints –
 Computational geophysics – Numerical modelling

#### 26 1 INTRODUCTION

During the last decade, seismic full waveform inversion has become a powerful and an increasingly 27 popular technique for Earth imaging (Tarantola & Valette 1982a,b; Virieux & Operto 2009; Monteiller 28 et al. 2013, 2015). However, with this method, density is retrieved with a lower resolution compared to 29 seismic velocities or Lamé parameters, and is often not sufficiently reliable for interpretation. Recov-30 ery of density from seismic data alone is difficult and may require the utilisation of prior information 31 (Alemie & Sacchi 2011; Lines 1999). Gravity data inversion is the common way of retrieving densities 32 but has a poor depth resolution and thus needs additional constraints. In this context, complementarity 33 with seismic data has been recognized (Lelievre et al. 2012) as seismic tomography provides seis-34 mic velocity models that can be exploited jointly with gravity data for improved subsurface density 35 imaging. Another motivation to perform gravity inversion constrained by seismic modeling is that 36 densities inferred from compressional seismic velocity models through Nafe-Drake or linear scaling 37 relationships may be affected by significant uncertainties that can exceed 10% (Herceg et al. 2015). 38 One of our main motivations is thus to reduce significantly these uncertainties by recovering densities 39 through gravity field data inversion constrained by seismic velocities, thereby preserving physical and 40 structural similarities between seismic velocities and densities. 41 Another long-term goal is to refine existing density models at depth to get insights into the composition 42 and thermal state of the lithosphere and to confront inverted models with existing geological models. 43 In this perspective, we use teleseismic FWI (TFWI) tomography as a priori information to constrain

<sup>44</sup> In this perspective, we use teleseismic Fw1 (IFw1) tomography as a priori information to constrain

45 gravity inversion and to refine existing density models. Scaling laws provide useful information on

density from crustal compressional velocity  $(V_p)$  models (Brocher 2005) that can be used as prior in-

<sup>47</sup> formation to constrain solutions of gravity inversion at lithospheric scale. In this context, we exploit

the results of TFWI on data collected in the Western Pyrenees during the 2009-2014 PYROPE and IB-ERARRAY seismic experiments (Chevrot et al. 2014, 2015, 2018) to constrain the inversion of gravity data provided by the BGI/Bureau Gravimétrique International (International Gravimetry Bureau). A  $V_p$  seismic model has been obtained by full waveform of teleseismic P-waves recorded in the westernmost PYROPE transect (Wang et al. 2016) in a 3D slice crossing the gravity anomaly of Mauleon's basin. This 3D slice was involving the seismic profile surrounded by temporary seismic stations to constrain laterally the TFWI. In a previous study in this region, where the strongest gravity anomalies in France are present (Martin et al. 2017), we reconstructed density distributions with an unconstrained gravity inversion procedure but densities still remained poorly constrained at depth. A conclusion of that study was that further inversions were needed with additional constraints and prior information to provide robust images of deeper structures : without sufficient prior information, gravity inversion is heavily affected by non-uniqueness and the inverse problem suffers from rank deficiency. Here, we introduce supplementary structural similarity constraints in the gravity data cost function minimization. We formulate these similarity constraints via cross gradients (e.g., Gallardo & Meju (2003)) between density and  $V_p$  models to obtain 3D density models that are consistent simultaneously with TFWI results and gravity data. In a similar work but more focused on offshore basin modelling, Welford et al. (2018) performed 3D gravity modeling to obtain 3D density models constrained by structural models derived from seismic tomography. More recently, Darijani et al. (2020) obtained 2D density models through a 2D gravity inversion constrained by a 2D seismic model at the near surface scale via a clustering/petrophysical constraint approach as in Lelievre et al. (2012). In our study, we rely on a

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<sup>68</sup> 3D model coming from TFWI and therefore we do not need such petrophysical/clustering constraints. <sup>69</sup> We introduce implicitly those constraints via a Nafe-Drake scaling relationship between density and <sup>70</sup>  $V_p$ .

Similar ideas have been proposed in other related works by Saunders et al. (2005) in the con-71 text of resistivity inversion constrained by seismic data, and by Brown & Singh (2012) and Yan & 72 Garcia Juanatey (2017) for electromagnetic and magnetotelluric data inversion constrained by fixed 73 seismic structures. Using linear relations between seismic velocites and densities or cross-gradient 74 constraints between seismic velocities, densities and magnetic susceptibilities, Colombo & Stefano 75 (2007), Stefano et al. (2011), and Moorkamp et al. (2011) performed joint inversion of seismic, gravity 76 and electromagnetic data. In these earlier studies, seismic tomography relied essentially on ray-theory 77 methods. Blom et al. (2017) performed a joint full waveform/gravity data inversion for a global scale 78 application, and found that additional seismic velocity-density correlations or structural constraints are 79 needed to properly reconstruct density anomalies. Lin & Zhdanov (2019) used the joint seismic and 80 gravity data inversion to image a synthetic salt-dome model. The method is constrained by a Gramian 81

stabilizer applied to the gradient of seismic velocities and densities to increase the correlation between the different physical parameters of the inverse model or their spatial gradients. In Giraud et al.
(2019b), gravity data inversions were constrained by geological structural uncertainty using entropy
arguments.

This article is organized as follows. After introducing the geophysical and geological context of 86 this study, we describe in a second part our inversion methodology and the optimization process. We 87 then explain how to appropriately weight the different constraint terms involved in the cost function to 88 be minimized and we show the models obtained after inversion. Then we present solutions of two kinds 89 of gravity data inversions constrained by the  $V_p$  model: a 2.5D gravity data inversion of a 1D Bouguer 90 anomaly profile aligned with the seismic transect and a 3D inversion of the available gravity data in 91 the 3D slice area. For the 2.5D gravity inversion, the 2.5D prior model is built by taking a 2D vertical 92 section extracted from the 3D TFWI model and extended along either the direction perpendicular to 93 the seismic profile or along the strike of the Pyrenees. As expected, we show that both the width and 94 the strike of the anomalies influence the gravity response. However, the finite extent of the anomalies 95 has a more dominant contribution than the orientation of the strike. All our 2.5D tests show that the 96 lateral extension of the Mauleon's anomaly must be finite, with a width of about 30 km. We performed 97 a 3D inversion to laterally localize the density anomalies, the 2.5D not being able to do it. The 2.5D inversions helped us to estimate the order of magnitude of the hyperparameters of regularization and 99 to refine more quickly the range of the hyperparameters for the 3D inversions. Finally, we compare 100 the different inverted models that we obtained in the 2.5D and 3D cases and propose a preliminary 101 geological interpretation of our findings. 102

#### 103 2 GEOLOGICAL AND GEOPHYSICAL CONTEXT

#### **104 2.1 Geology of the area**

The Pyrenees result from the collision between Iberia and Eurasia from late Cretaceous to early 105 Miocene (Lescoutre 2019; Lescoutre & Manatschal 2020; Gómez-Romeu et al. 2019). Positive com-106 plete Bouguer gravity anomalies characterize the northern flank of the Pyrenees, which are particularly 107 strong in the Mauleon basin and close to the town of Saint-Gaudens (section A-A' in Figure 1-a). Un-108 derstanding the nature and origin of these anomalies (from the upper mantle or from shallow crust 109 structures) has been a long-lasting controversy, and was one of the main motivations of the PYROPE 110 and IBERRARRAY seismic deployments from 2009 to 2014 (Chevrot et al. 2014, 2015), and of the 111 later OROGEN deployments from 2015 to 2017 (Chevrot et al. 2018). Another motivation for study-112 ing the western part of the Pyrenees is that this region is seismically more active than the eastern part 113

(Souriau & Pauchet 1998). In particular it presents a pronounced concentration of seismicity beneath 114 the northern Pyrenean foothills that is not observed in the eastern Pyrenees. This feature may be related 115 to the strong structural asymmetry of the Pyrenees, with a continental subduction in the central and 116 western Pyrenees that is absent in the eastern Pyrenees (Chevrot et al. 2018). Recently, FWI has been 117 applied to teleseismic P waves recorded along the westernmost PYROPE profile, complemented with 118 data recorded by nearby permanent stations. The resulting 3D  $V_p$  model (Figure 2), which resolved the 119 structures over a band of 60 km sourrounding the profile, revealed the presence of a shallow mantle 120 body at 10 km depth below the Mauleon basin (Wang et al. 2016; Martin et al. 2017; Chevrot et al. 121 2018). This mantle body, probably exhumed during the Cretaceous episode of rifting, explains the 122 large positive Bouguer anomalies shown in Figure 1-b. 123

As mentioned in Martin et al. (2017), FWI can provide compressional and shear velocities as well as densities but in practice density is not really well reconstructed by FWI alone (Wang et al. 2016; Beller et al. 2017). Therefore, adding gravity data into the inversion can improve the density model reconstruction. Here, we aim at inverting a complete Bouguer gravity anomaly data set extracted from the BGI database under the constraint of a  $V_p$  model obtained by inverting teleseismic P waveforms recorded by the westernmost PYROPE profile (Chevrot et al. 2015).

#### **2.2** Geophysical data and prior information for inversion

To perform gravity inversion constrained by compressional velocity models, we consider the dense 131 (65062 points) complete Bouguer gravity anomaly dataset from the BGI database covering the French 132 and Spanish continental regions (see the map of measured Bouguer gravity data in Figure 1a). These 133 data have been used to obtain a 2 mn arc gridded global model of the complete Bouguer gravity 134 anomalies (Balmino et al. 2012; Geodesist's-Handbook 2012) shown in Figure A1. For our study we 135 prefered to use directly the measured data instead of the gridded data in order to make computations 136 at the measurement points for maximum accuracy in the calculations. From this measured dataset, we 137 extract a subset of 13000 points that are projected on a regular 2700 ( $135 \times 20$ ) points grid (340 km 138 long  $\times$  50 km wide and rotated 45° eastward) that includes the westernmost (A-A') 2.525 km reso-139 lution transect imaged by TFWI (See Figures 1b and 1c). This seismic profile runs from coordinates 140 (-2.615°, 42.071°) to (0.32167°, 44.4323°) and crosses the Ebro and Mauleon basins. Those 2700 141 gravity data points, located up to 25 km from the transect are used for 3D inversion and are also inter-142 polated along this profile (136 points with a 2.525 km spacing) for 2.5D inversion. Along the profile, 143 gravity anomalies show strong variations across the Pyrenees with anomalies, varying between -90 144 mgal in the south to +30 mgal in the north. 145

<sup>146</sup> We now define the 3D a priori density model of the western Pyrenees that will be used in our

Bouguer anomaly inversions. The density model is first constructed by extracting a  $V_p$  volume around the seismic profile mentioned before. We scaled the a priori density model  $\rho$  using this  $V_p$  model and using the Nafe-Drake law (Nafe & Drake 1957; Ludwig et al. 1970; Brocher 2005) as in Martin et al. (2017):

$$\rho = 1.6612V_p - 0.4721V_p^2 + 0.0671V_p^3 - 0.0043V_p^4 + 0.000106V_p^5, \text{ for } V_p < 7.4 \text{ km/s}$$
(1)

and

$$\rho = \rho_m = 3270 kg/m^3, \text{ for } V_p > 7.4 \text{ km/s}$$
(2)

We define the density anomalies  $\Delta \rho = \rho - \rho_c$  in the crust (from the upper surface down to a 151 reference Moho depth of 30 km) as the deviation from a reference crustal density  $\rho_c = 2670 \text{ kg/m}^3$ , 152 and  $\Delta \rho = \rho - \rho_m \, \text{kg/m}^3$  beneath the Moho for a reference upper mantle density  $\rho_m$  (at depths larger 153 than 30 km). The 3D prior density model is shown Figure 3 with different cut sections at different 154 depths (16.4 km, 50 km). Predicted Bouguer gravity anomalies (Figure 1-b) are relatively close to the 155 measured Bouguer anomaly in the central and northern part of the profile. In our numerical tests, we 156 have also observed that computed gravity responses are not influenced by density structures located 157 farther than 25 km from the transect. As in Martin et al. (2017), a 340 km long  $\times$  50 km wide  $\times$  75 158 km deep 3D inner computational domain is considered and discretized over  $136 \times 20 \times 30$  prismatic 159 bodies (2.525 km  $\times$  2.525 km  $\times$  2.533 km volume per cell). An external tapering is added to the inner 160 computational domain (see Figure 5) in order to avoid edge effects. It involves 20 extra cells on each 161 vertical outer interface of the computational domain. The 1 mn arc ( $\approx 1.78$  km) ETOPO1 topography 162 is added and interpolated at a resolution of 2.525 km resolution in longitude and latitude on top of the 163 computational mesh. The gravity measurements are projected on this topography grid (Figures 4 and 164 5). Furthermore, the computational mesh is distorted close to the surface to follow the topography. 165

The 2.5D models are built by extracting 2D  $V_p$  and density sections from the 3D TFWI models 166 along the transect and by replicating them invariantly to themselves over a 30 km (Figure 6-A) or a 167 44 km width (Figure 6-B). They are rotated with different angles  $\theta$  with respect to the A-A' profile 168 from 0 degree, which corresponds to the direction perpendicular to A-A' (line P-P') to 45 degrees 169 which corresponds approximately to the strike of the Pyrenees (S-S' in Figure 4). In Figure 6, we 170 show the influence of the angle of rotation and width of different 2.5D a priori models on the gravity 171 response. For a 44 km width, the gravity anomalies are overestimated by a large amount for all angles 172 of rotation (Figure 6-B), while for a 30 km width the gravity anomalies are in good agreement with the 173 observed data. For a 30 km width and angles of 0 to 25 degrees, the amplitudes are very similar and are 174 overestimated by 2-4 mgals while for 45 degrees they are underestimated by 2 mgals approximately. 175

This suggests that the strong anomaly produced by the shallow mantle body beneath the maximum gravity anomaly is oriented along a direction close to the strike of the Pyrenees (at an angle between 30 and 40 degrees from the P-P' transect). This width and those angles are close to those estimated ( $\simeq 24$  km width) at the the first order by Wang et al. (2016). However, note that for narrow density anomalies their orientation has a secondary effect compared to their lateral extent.

#### **181 3 STRUCTURALLY CONSTRAINED INVERSION METHOD**

Starting from a Nafe-Drake scaled density model as defined in the previous section, we explain now
 to perform the gravity data inversion under structural similarity constraint of densities by minimizing
 the cross-gradient between density and a fixed seismic velocity model obtained from TFWI.

#### **185** 3.1 Structural constraints

In our constrained inversion, structural correlations are taken into account between density anomalies  $\Delta \rho$  and compressional velocites  $V_p$ . We assume that at any point in the medium there exists, to first order, a spatially varying parameter  $\beta$  such that  $\nabla \Delta \rho = \beta \nabla V_p$ . Here, we consider the  $V_p$  model obtained through TFWI as a suitable structural model describing the deep crustal architecture.

The structural constraints we apply here consist of minimizing the cross-gradient between density and velocity anomalies similarly to the joint resistivity-velocity inversion procedure used by Gallardo & Meju (2003) and by many others since then (Meju & Gallardo 2016). Imposing a zero cross-gradient between two model distributions is equivalent to imposing local colinearity between the spatial gradients of the two models. The advantage of using the cross-gradient in our study is that we do not need to impose any predefined linear correlation function or any coefficient  $\beta$  in the inversion.

#### **196 3.2** Inverse problem formulation and resolution

Let us now describe our methodology for gravity data inversion under seismic constraints. We minimize a cost function  $\chi$  that involves the misfit between measured and computed complete Bouguer gravity anomalies, and regularize the problem by adding a damping of the norm of the density anomaly model  $\Delta \rho$  and a structural constraint using the cross-gradient between density and  $V_p$  models. The total cost function is thus

$$\chi(m) = || D_{obs} - D_{cal} ||_{l^2}^2 + \lambda^2 || W(\Delta \rho - \Delta \rho_p) ||_{L^2}^2 + \alpha^2 || \nabla \Delta \rho \wedge \nabla V_p ||_{L^2}^2,$$
(3)

where  $\Delta \rho$  is the density anomaly,  $\Delta \rho_p$  the prior density anomaly,  $D_{obs}$  and  $D_{cal}$  the measured and theoretical Bouguer gravity data, and  $\lambda$  and  $\alpha$  the regularization weights applied to the density model and the cross-gradients respectively. W is a depth weighting operator applied on the model and computed by integrating the sensitivity gravity kernel S over the whole mesh volume and for each observation point location (Portniaguine & Zhdanov 2002). For the density anomaly in cell k of the computational mesh, this matrix operator W is defined as

$$W_{kk} = \sqrt{(\sum_{i=1,Nobs} S_{i,k}^2)^{1/2}},\tag{4}$$

<sup>197</sup> where  $S_{ik}$  is the element of the gravity kernel S linking the density anomaly  $\Delta \rho_k$  in cell k to the <sup>198</sup> gravity anomaly  $D_{cal}^i$  at location  $x_i$  such that  $D_{cal}^i = S_{ik} \Delta \rho_k$ .

The cross-gradient is discretized in space using a finite-difference scheme. In our Tomofast-x parallel inversion platform, we minimize Equation (3) using the LSQR algorithm of Paige & Saunders (1982), which is implemented using a parallelized sparse matrix solver. At each inversion cycle (i.e., outer loop of LSQR inversion), the model is updated using an approximate solution using a fixed number of iterations in the inner loop of the LSQR algorithm (Martin et al. 2013, 2018; Giraud et al. 2019a,b).

#### **4 NUMERICAL RESULTS OF THE STRUCTURALLY CONSTRAINED INVERSION**

#### **4.1** Weighting of cost function terms in the 2.5D and full 3D inversion cases

To minimize the aggregate cost function (3) it is crucial to achieve optimum balancing between the different contributing terms. We determine the optimum weights  $\lambda$  and  $\alpha$  following a L-curve approach (Hansen and O'Leary, 1993), which we extend to the two-parameter case by using a strategy similar in spirit to the Pareto optimization scheme (Bijani et al. 2017).

Our analysis is based on the minimization of the data misfit cost function (term 1 in equation 211 (3), Figure 7-a), the model norm (term 2 in equation (3), Figure 7-d), cross-gradient norm (term 3 in 212 equation (3), Figure 7-c) and the aggregate global cost function  $\chi$  in equation (3), black solid curve in 213 Figure 7-e). In Figure 7-b, we show the behavior of the cross-gradient and the model norms for a low 214 data misfit of  $10^{-4}$ . We estimate the optimum ( $\lambda, \alpha$ ) values by identifying the inversion case fulfilling 215 a series of conditions in terms of data misfit (Figure 7-a), model norm (Figure 7-d), and cross-gradient 216 (Figure 7-c) values. The method has been applied to the four 2.5D a priori models rotated by 0, 20, 25 217 and 45 degrees respect to the P-P' direction. Similar inverted solutions have been obtained in the four 218 cases and similar  $(\lambda, \alpha)$  regularization parameters have been obtained. We describe now how those 219 hyperparameters have been obtained for the 2.5D case (for 0 degrees for instance) and also for the 3D 220 inversion and we present and compare the 2.5D and 3D results. 221

The process to determine  $\lambda$  and  $\alpha$  is divided in three main stages. We first analyse a population

of inverted models obtained from inversions using a range of values sampled on a discretized ( $\lambda, \alpha$ ) 223 grid. To accelerate the search, we take a 2.5D a priori model averaged along the (A-A') transect that 224 is extended invariantly to itself over 12 cells perpendicularly to the right and left of the profile. In our 225 study, the  $(\lambda, \alpha)$  grid consists of 11 x 11 values and is used to generate a collection of 121 inverted 226 models. In a second stage, from this set of models, we then define a refined subrange of values thought 227 to contain the optimum ( $\lambda$ ,  $\alpha$ ) pair. In this refined subrange, here taken as  $[10^{-8}, 5 \ 10^{-5}] \times [10^{-5}]$ , 228  $10^{-1}$ ], we refine the weights sampling around the optimal values. To this end, we perform 21 x 19 229 inversions on a refined set of  $(\lambda, \alpha)$  pairs. 230

The estimate of the optimum set of weights (see Figure 7-a) that balance the contribution of 231 the different terms is obtained by identifying the case with lowest overall cost among the subset of 232 inverted models honoring all the conditions (see Figure 7-e). In these 2.5D inversions, we choose a 233 damping model parameter  $\lambda = 3.5 \times 10^{-7}$  and a cross gradient weight  $\alpha = 2.3 \times 10^{-4}$ . To ensure 234 appropriate balancing between the different terms of the cost function, the optimum weights of the 235 different terms have been inferred from the inflection points in the curves of data misfit curve versus 236 model perturbations and cross-gradient norm (Figures 7-b,c,d). We apply the L-curve analysis by 237 performing many inversion runs with different  $\lambda$  and  $\alpha$  values. An example is taken along the dashed 238 lines shown in Figure 7-e where the optimum  $\alpha$  value is determined and fixed and an optimum  $\lambda$  value 239 is determined accordingly. In a third stage, once the optimal values of the damping model parameter 240  $\lambda$  and of the cross gradient weight  $\alpha$  have been found in 2.5D, we perform the inversions over the 241 full 3D heterogeneous model with values of  $\lambda$  and  $\alpha$  finely tuned around the values obtained in the 242 previous 2.5D case. 243

# 4.2 Cross-gradient constraints and their influence on density model reconstruction : the 2.5D case example

To show the impact of an a priori model and the different penalty terms of the misfit function on the 246 inverted solutions, we performed different tests with or without damping or cross-gradient penalty 247 in the misfit function. For the sake of clarity, the results of constrained and unconstrained inversions 248 are described in appendix B for the 2.5D model example (i.e for an a priori 3D model defined as a 249 Nafe-Drake scaled density model extrapolated in the direction P-P' orthogonal to the A-A' profile). 250 As shown in Figure A2, the data misfit function is well minimized in all cases, which suggests that 251 the solution of the inverse problem is not unique. To obtain physical solutions at depth, as discussed 252 in appendix B and observed in figure A3, it is thus crucial to perform the inversions considering 253 all the terms of the total cost misfit function. We now focus our attention on the inverted solutions 254 obtained under constraints. In Figure 9 we show the differences between inverted solutions obtained 255

for the prior density model extracted from the TFWI model and extrapolated invariantly to itself in 256 directions making an angle  $\theta$  with the transect P-P' perpendicular to the A-A' profile. For  $\theta=0$ , the 257 model is invariant in the direction P-P' and for  $\theta = 45$  degrees it is invariant along the S-S' direction 258 parallel to the strike of the Pyrenees passing through the highest Mauleon's gravity anomaly. As we 259 can see, the differences are rather small, with maximum absolute differences and standard deviations 260 of approximately 4 and 1.5 kg  $m^3$  obtained for the 45 degrees case. The solutions are very close with 261 a small but noticeable difference close to the surface. Again, these small differences result from the 262 limited lateral extent of the anomalies as it was already the case for the responses of the four a priori 263 models used in those 2.5D inversions. 264

For the 2.5D density modeling case, we first minimize the misfit cost function without the cross-265 gradient term and we obtain a density distribution that is not well constrained at depth (Figure 8) as 266 in Martin et al. (2017). As already mentioned, instead of normalizing the sensitivity matrix by a depth 267 weighting function, we use the integrated sensitivity technique of Portniaguine & Zhdanov (2002). The 268 differences between inverted and prior density models are shown in Figure 8. The solution is obviously 269 not geologically relevant because the model perturbations are mainly concentrated close to the surface 270 and decrease continuously with depth. To alleviate this, we take the same prior model and we now 271 minimize the cost function with the cross-gradient constraint. This time, we obtain well constrained 272 densities at depth with density perturbations that follow the spatial variations of the  $V_p$  model (see the 273 evolution of the cross-gradient in Figure 10). After 200 successive inversion cycles, the cross gradients 274 are minimized in the first 60 km depth. In the first inversion cycles, the cross gradients are strong, but 275 they progressively decrease and tend to very low values not only close to the surface but also at depth. 276 Note that the differences between a priori and inverted densities are as pronounced at depth as they 277 are closer to surface (Figure 8-bottom). We note that this feature is not possible to achieve without 278 geometrical/structural constraints. In Figure 7-e we can see the evolution of the different terms of the 279 whole cost function that reaches a value of  $10^{-7}$  after 20 successive LSQR inversions (outer loop) with 280 300 iterations for each LSQR inversion. At the end of the inversion the cost function reaches a value 281 of approximately  $4 \times 10^{-8}$  and the data misfit has decreased by more than 80% (see Figure 7-e). The 282 2.5D inversion helps to tune the penalty parameters. However, it does not take into account correctly 283 nor the localization of the lateral heterogeneities neither their orientation in the vicinity of the A-A' 284 profile. It tends to concentrate the density perturbations along the central profile due to a different 285 geometrical divergence of the gravity fields and also to decrease the density anomaly values below the 286 location of strong gravity anomalies. It is thus always preferable to perform a full 3D inversion that 287 allows to localize the density anomalies below strong gravity anomalies are present and also to better 288 define their orientation. 289

In order to have better images in the direction perpendicular to the profile, we perform gravity in-291 versions for  $\alpha$  and  $\lambda$  values ( $\lambda = 2 \times 10^{-7}$  and  $\alpha = 10^{-3}$ ) close to the optimal values obtained 292 previously in the 2.5D case. As starting and a priori model we take the density model scaled with the 293 3D  $V_p$  model obtained by FWI according to the Nafe-Drake law. The inner computational domain is 294 the same as previously. However, a padding of 20 cells has been added to each outer vertical edge of 295 the model to avoid edge effects. The 3D model has thus a total size of  $175 \times 60 \times 30$  grid points. 296 We perform 100 LSQR inversion cycles (outer loop) to achieve enough convergence of the whole in-297 version algorithm until reaching a total cost function value of  $3.6 \times 10^{-7}$ . Gravity data are very well 298 reproduced with point-to-point absolute errors lower than 0.4 mGal ( $4 \times 10^{-6}$  m/s<sup>2</sup>), a total data misfit 299 contribution of  $5.46 \times 10^{-8}$  to the total misfit function, and a global relative error of  $2.235 \times 10^{-3}$ . 300 Figure 12 shows the final model along the A-A' profile in a vertical section and also in a horizontal 301 plane located at a 16.4 km depth (Figure 12-a), as well as in a section P-P' perpendicular to the profile 302 (in the direction of the axis of the Pyrenees, Figure 12-d). Inverted densities are showing variations of 303 +/- 130 kg/m<sup>3</sup> slightly higher than to those obtained for the 2.5D inversion (+/- 100 kg/m<sup>3</sup>). Density 304 anomalies close to the Moho are showing clear subduction of the Iberian plate beneath the European 305 plate (negative density anomaly below 30 km depth) with part of the European Mantle rising up close 306 to the surface (strong positive anomaly above the 30 km reference Moho depth). Indeed, in Figure 12, 307 the new model emphasizes the subduction of the Iberian plate (represented by a strong negative den-308 sity anomaly in blue) and the presence of exhumed mantle material (evidenced by a positive anomaly, 309 high red values) reaching a  $\simeq 10$  km depth. In the section perpendicular to the Pyrenean axis (Figure 310 12-d), the 3D inversion constrains the width of the exhumed mantle body to about 20 km in agree-311 ment with the 2.5D inversions (Wang et al. 2016). However, the 3D full modeling provides a better 312 reconstruction of the geometry of the anomalies in particular of the shallow mantle body, with better 313 localization, orientation, and more accurate width. Furthermore, the exhumed anomaly can be located 314 laterally, which is not possible by construction in the 2.5D configuration. This can be observed in 315 Figure 12-a on the section located at a depth of 16.4 km, where the exhumed mantle anomaly is not 316 exactly on the A-A' axis but is rotated with an angle of about 45 degrees with respect to P-P' direction. 317 The remaining differences between inverted and a priori models are mainly observed in the Iberian-318 European collisional domain. The initial cross-gradients are lower than those of the 2.5D case by an 319 order of magnitude everywhere. Below 20 km depth, they are decreasing from about  $4 \times 10^{-3}$  down 320 to  $1.5 \times 10^{-3}$  after inversion. At 5-10 km depth, cross-gradients are also reduced but remain important 32 on top of the exhumed mantle body. In general, gravity data alone allow us to recover densities close 322

to the surface but not at depth. But, thanks to the cross-gradient, we can also constrain deep density anomalies.

In Figure 13, a dispersion diagram between density and  $V_p$  is shown for constrained and uncon-325 strained solutions, and compared with the Nafe-Drake reference scaling. As in Martin et al. (2017), 326 the densities obtained without  $V_p$  similarity constraints are overestimated and density values lower 327 than 2550 kg/m<sup>3</sup> are almost absent close to the surface level and at depth. Moreover, adding the cross-328 gradient constraint increases the amplitude of the variations of the densities compared to the densities 329 obtained without cross-gradient constraints: it decreases further the densities where anomalies are neg-330 ative close to the surface and also at depth until reaching the crust-mantle transition. This reduction 331 has an amplitude ranging between -130 and +130 kg/m<sup>3</sup>. We now obtain lower densities in the crust 332 and close to the surface in agreement with the results of Grandjean (1994) in which densities are lower 333 than  $2500 \text{ kg/m}^3$  in the first 7 km in the basins. 334

#### 335 5 GEOLOGICAL AND GEOMECHANICAL INTERPRETATION

Visually, the recovered density model bears important similarities with the tomographic model of 336 Wang et al. (2016), as can be seen in Figure 14. The model is also coherent with the recent collision 337 models of Lescoutre (2019) (chapter III, Figure p.121, and Figure III-4, p. 131) and Lescoutre & 338 Manatschal (2020); Gómez-Romeu et al. (2019). Our inversions show that the European mantle wedge 339 and the Gavarnie nappe have strong imprint in the density model, with strong negative and positive 340 density contrasts respectively (see Figure 12-c-left). The exhumed mantle body and the Gavarnie thrust 341 show geometries in good agreement to the northern part of their transect passing through the Eastern 342 part of Mauleon basin (profile A in Lescoutre (2019), Chapter III, Figure p.121). The southernmost 343 part of our model is more similar to the geological profile passing through the west of Mauleon basin 344 (profile B in Chapter III, p.121 Lescoutre (2019), reproduced in appendix A.5). Again, this simply 345 results from the strong obliquity of the seismic transect with respect to the strike of the Pyrenees. Our 346 3D imaged section corresponds also to the profile passing through the Ebro basin and eastern Mauleon 347 (section in of Figure III-4 of Lescoutre (2019), p. 131) and reproduced also in Figure A.5. In short, 348 the AA' model profile (Figure 1) can be seen as an intermediate stage between these two south-north 349 transects : one passing through the Eastern Mauleon basin and another one passing through Saint-Jean 350 de Luz basin and Ebro basin at the west of Mauleon basin, with a central part where the geometry of 351 the mantle body is in good agreement with Wang et al. (2016). 352

We computed the Airy isostatic gravity anomalies by taking a reference Moho model obtained by assuming a 30 km compensation depth and topography interpolated form a ETOPO1 (1mn resolution). Reference isostatic densities of 2670 kg/m<sup>3</sup> above this Moho and 3270 kg/m<sup>3</sup> beneath are used. In Figure 15, the observed isostatic anomalies are very similar to the isostatic anomalies computed in the final density model (i.e after inversion). The isostatic anomalies are reduced in the southern part of the profile compared to the Bouguer anomalies due to surface topography which predicts a deeper Moho (reaching around 36 km depth) that partly compensates the topography in that region, which is not the case in the northern part. The differences between observed and calculated anomalies are very small and reach maximum errors lower than 1 mGal (as can also been seen in Figure 12-d). This comparison demonstrates that it is equivalent to invert either Bouguer or isostatic anomalies.

#### 363 6 CONCLUSIONS

We have performed 2.5D and full 3D gravity data inversions in the region showing the strongest gravity 364 anomalies in the Pyrenees using structural constraints derived from a tomographic  $V_p$  model to favor 365 structural similarities between seismic velocity and density models. These constraints improved the 366 density models at depth, by transferring structural information from TFWI to the density model, and 367 providing structural details of the mantle wedge and the upper crust structures. Full 3D inversions with 368 topography allow us to take into account lateral variations of densities and to localize heterogeneities 369 at depth more accurately than with 2.5D inversions. 3D inversions also tend to better define their 370 orientation (along the strike of the Pyrenees), whereas 2.5D inversions tend to decrease anomalies and 371 concentrate them closer to the surface and along the central plane. The structural constraints adjust 372 the densities not only close to the surface but also at depth close to the Moho with up to 10% density 373 variations. However, 2.5D inversions allow us to tune quickly a range of penalty parameters of the 374 cost function that can be used to estimate penalty hyperparameters for the full 3D inversions. These 375 3D inversions can be run in less than 20 minutes on 256 Intel Skylake 2.3GHz cores of the Olympe 376 supercomputer. Inverting Bouguer or isostatic anomalies can be equivalently done and gives similar 377 density models. They only differ by a shift generated by the removal of the reference Moho depth 378 perturbation from the Bouguer anomalies. 379

In a future and second step, our methodology will be applied in 3D to the rest of the Pyrenees. 380 Future work will include joint cross-gradient inversion of gravity and seismic data at the scale of 381 the whole Pyrenees. We will also consider adding constraints such as petrophysical and geological 382 information as in Wehr et al. (2018). In the present study, we performed inversions on medium sized 383 supercomputing resources (50 to 200 processors clusters) but for the inversion of the whole Pyrenees 384 area much more processors will be needed (at least 10 to 20 times more). In the mid-term, having 385 access to the densities will provide key information on the mineralogic composition and thermal state 386 of the lithosphere. To this end a full joint inversion seems to be a promising way to improve our 387 capacity to image internal Earth structures by reducing model uncertainties. 388

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**Figure 1.** (a) Measured Bouguer gravity anomaly data in Southwest France and North Spain. The western transect seismic profle A-A' crossing the Mauleon and Ebro basin in the Pyrenees close to Labour town (Chevrot et al. 2018) is shown in blue. (b-middle) Observed (black solid) and a priori (blue solid) Bouguer gravity anomalies close to the westernmost transect A-A'. (c)  $V_p$  and Nafe-Drake scaled prior density model  $_rho$  along the A-A' profile.



**Figure 2.** 3D  $V_p$  model along the A-A' profile at 16.4 km (left column) and 50 km depth (right column). Sections perpendicular to the A-A' profile are shown too at x = 200 km (top), 226 km (middle, where the exhumed mantle is going up close to the surface) and 290 km.



NW-SE axis [km]

**Figure 3.** 3D Nafe-Drake scaled prior density model  $\rho$  along the A-A' profile at 16.4 km (left column) and 50 km depth (right column). Sections perpendicular to the A-A' profile are shown too at x = 200 km (top), 226 km (middle, where the exhumed mantle is going up close to the surface) and 290 km.

NW-SE axis [km]



**Figure 4.** Top view of the measured/not gridded data is shown (left) as well as the data interpolated (right) in the region of interest (inside the black box) containing the (A-A') seismic profile (red line). The interpolated data are gridded at 2.471 km resolution. The line segment P-P' perpendicular to the seismic profile and the Pyrenean strike segment S-S' passing through the Mauleon's gravity anomaly are shown. Both segments make an angle  $\theta$  around 40 degrees.



**Figure 5.** Bouguer gravity anomaly interpolated on the topography in the computational slice of interest. ETOPO1 1 mn arc resolution topography interpolated at 2.471 km resolution is considered in the computational area of interest that includes the (A-A') seismic profile. The computational mesh used for data inversion takes into account the topography. The first layer of the computational mesh is distorted, follows the topography and is also shown on the figure. Lateral padding of the computational model is added, taking into account the topography outside the set of gravity data (in color).



**Figure 6.** (a)Bouguer gravity anomalies are shown for the a priori 2.5D model extracted from the 3D TFWI model, interpolated at 2.471 km resolution along the (A-A') seismic profile and replicated invariantly to itself over a width of 30 km. Four cases are plotted : in the direction perpendicular to the profile (angle  $0^{\circ}$ ) or rotated by an angle ( $20^{\circ}$ ,  $25^{\circ}$ ,  $45^{\circ}$ ) respect to the profile. The a priori anomalies are very similar and are comparable to the observed field anomalies. (B) Same thing as in Figure A but for a 44 km width of the density anomalies. We can observe that the anomalies are overestimated when compared to the 30 km model width case with or without rotation of the model.



Figure 7. Data misfits are normalized by the sum of squared data. (a-Top) 3D representation of the three terms of the cost function. The optimal regularization parameters are indicated by the black dot. (b-Top) Section of this surface passing through this point. (c and d : Middle left and right) *L* curves to define the optimal model regularization and cross-gradient weights respectively corresponding to the optimal model damping and cross-gradient terms shown in Figure (a). Refined subrange of weighting parameters ( $\lambda$ , $\alpha$ ) varying in the set intervals  $[10^{-8}, 5 \ 10^{-5}] \times [10^{-5}, 10^{-1}]$  has been used. (e-Bottom) Evolution of data misfit, cross-gradient and model damping norms through inversion iterations.



**Figure 8.** Difference between inverted and prior density models in the 2.5D ('quasi 3D') case. (Top) Without cross-gradient constraint, and without (a) or with (b) starting model. (Middle) With cross-gradient constraint, and without (c) or with (d) starting model. Strong differences are appearing at depth, with variations exceeding + or  $-100 \text{ kg/m}^3$ , particularly when cross-gradient constraint is applied. Note also that differences are predominantly vertical. (Bottom-e) Observed and inverted gravity data with and without cross-gradient constraint.



**Figure 9.** We show the standard deviation (Figure a) as well as the difference per cell between the maximum and minimum density values (Figure b) over all the four inverted models obtained for the prior models rotated by an angle of 0, 20, 25 and 45 degrees in the trigonometric sense respect to P-P' transect. Minimum and maximum values of + or -4 kg/m<sup>3</sup>, and maximum standard deviations of around 1.7 kg/m<sup>3</sup> are reached. There is not any significant difference between the inverted models. In Figure c the inverted gravity data are shown for the four cases with the different angles : there is almost no differences between them.





**Figure 10.** (Left) From top to bottom : cross-gradient evolution for 5, 10, 50, 100 and 200 inversion loops. Cross-gradient is decreasing as expected. (Right) Inverted effective densities with cross-gradient constraints.





**Figure 11.** 3D inverted density model  $\rho$  along the A-A' profile at 16.4 km (left column) and 50 km depth (right column). Sections perpendicular to the A-A' profile are shown too at x = 200 km (top), 226 km (middle, where the exhumed mantle is going up close to the surface) and 290 km.



**Figure 12.** Full 3D gravity data inversion results. (a) Left: Density model along the (A-A') profile at 16.4 km depth. Right: Difference between inverted and prior Nafe-Drake scaled model. (b) Left: vertical inverted density model section along A-A' profile. Right: Difference between inverted and prior Nafe-Drake model. (c) Left: Vertical density anomaly section (relative to the 2670 kg/m<sup>3</sup> crust and 3270 kg/m<sup>3</sup> Moho density reference model) along A-A' profile. Right: Difference between inverted and starting model. (d) Left: Vertical inverted density section along the Pyrenean axis perpendicular to A-A' transect. Right : Observed and inverted gravity data differences (lower than 0.4 mGal) on topography. (e) Cross-gradient before (left) and after (right) inversion.



Figure 13. Dispersion diagram of  $\rho/V_p$  properties around the initial  $\rho/V_p$  Nafe-Drake scaling relation with and without seismic constraints. The correlation between inverted density and  $V_p$  models obtained after gravity data inversion constrained by seismics is shown in red (blue for the non-constrained inversion case). When compared to the non-constrained densities, the seismic constrained densities are lowered close to the surface and also at depth, in the northern part of the section and in the diping part of the Iberian crust.



**Figure 14.** Zoomed density after inversion overlaid with geological interpretation of tomographic model from Wang et al. (2016) for the 2.5D case (Figure a) and the full 3D case (Figure b)



**Figure 15.** Difference between observed and computed (after inversion) isostatic anomalies for a reference Moho computed with a 30 km compensation depth.

#### 502 APPENDIX A: INVERSION ALGORITHM

<sup>503</sup> A least-squares algorithm is used here to solve the matrix system as follows. Let us denote m the <sup>504</sup> model vector containing the density anomalies  $\Delta \rho$ . This model vector is obtained by solving the <sup>505</sup> linear system of equation

$$\begin{bmatrix} SW^{-1} \\ \lambda I_d \\ \alpha W^{-1} \nabla V_p \wedge \nabla \end{bmatrix} [Wm] = \begin{bmatrix} \Delta g_{obs} \\ \lambda Wm_p \\ 0 \end{bmatrix},$$
(A.1)

where  $m_p = \Delta \rho_p$  is the a priori model and the gravity kernel *S* is depth-weighted by the operator *W* given in equation (4). The solution of (A.1) is obtained by an iterative LSQR algorithm (Paige & Saunders 1982). At each *i*-th LSQR inversion cycle we solve the following linearized version of the system of equations (A.1)

For 
$$1 \leq i \leq Niter_{max}$$
  

$$\begin{bmatrix} SW^{-1} \\ \lambda I_d \\ \alpha W^{-1} \nabla V_p \wedge \nabla \end{bmatrix} \begin{bmatrix} \Delta \overline{m}^i \end{bmatrix} = \begin{bmatrix} \Delta g_{obs} - \Delta g(m^{i-1}) \\ -\lambda W(m^{i-1} - m_p) \\ -\alpha \nabla V_p \wedge \nabla m^{i-1} \end{bmatrix}$$

$$\Delta m^i = W^{-1} \Delta \overline{m}^i$$

$$m^i = m^{i-1} + \Delta m^i$$
End for , (A.2)

where  $Niter_{max}$  is the maximum number of outer loop inversion cycles. Spatial gradients are computed using forward finite difference integration in the computation domain and using backward finite difference integration at the outer boundaries.

# APPENDIX B: INFLUENCE OF INITIAL MODELS AND PENALTY CONSTRAINTS ON DENSITY MODEL RECONSTRUCTION : DATA AND MODELS WITH OR WITHOUT STARTING MODELS, DAMPING REGULARIZATION AND CROSS-GRADIENT CONSTRAINTS.

Let us first consider the impact of an a priori model, a damping term on the model or a cross-gradient in the misfit function. As an example we consider the 2.5D model case (i.e for a 2D model defined as a Nafe-Drake scaled density model and extrapolated in the direction orthogonal to the A-A' profile). As shown in Figures A2, the data misfit function is well minimized in all cases, which suggests that the solution of the inverse problem is not unique. Figure A3 shows the effective density models and

- the difference with the a priori model (scaled from the  $V_p$  model using a Nafe-Drake law) or a density model of reference. In Figures 8 and A3, the inverted solutions are represented for inversions with and without starting models in the following cases :
- Case 1 : without damping ( $\lambda = 0$ ) and without cross-gradient ( $\alpha = 0$ )
- Case 2 : with damping  $(\lambda \neq 0)$  and without cross-gradient  $(\alpha = 0)$
- Case 3 : without damping ( $\lambda = 0$ ) and with cross-gradient ( $\alpha \neq 0$ )

where the non zero parameters  $\lambda$  (case 2) and  $\alpha$  (case 3) are chosen for clarity as the optimal values ( $\lambda = 5 \times 10^{-7}$  and  $\alpha = 2.3 \times 10^{-4}$ ) defined using the method described in the previous section.

Figure A2 shows the fit to gravity data obtained after inversion with or without starting model, with or without damping model regularization, and with or without cross-gradient constraints. Figure A3 shows the different density models obtained with the different types of inversions.

In Figures 8a-b and A3a-b, the case 1 is treated without or with a starting model. In the reconstructed model, the strongest density anomalies concentrate close to the surface where the highest gravity anomalies are present. This example illustrates that gravity inversion has a poor depth resolution. However, a better reconstruction of density anomalies close to the surface is achieved when a starting model is introduced (Figures A3c).

In case 2, densities are computed at depth with or without starting model and are exhibiting strong similarities (see Figures A3d-e). The solution is very close to the one obtained in case 1 when a starting model is introduced and no damping term is involved (see also Figure 8c). This result suggests that the damping term acts as a depth-dependent preconditionner of the matrix system (A.1) but the starting model does not prevent the inversion from concentrating the anomalies close to the surface.

In case 3 (Figure A3-f), the cross-gradient term adjusts the densities at depth to follow the varia-543 tions of the  $V_p$  model. But, as it is the case here, if no physical Nafe-Drake scaled starting model or 544 if no damping term based on this prior model is introduced, these density variations are not following 545 successfully the  $V_p$  variations at depth, more specifically close to the crust-mantle transition (between 546 30 and 40 km depth). The inverted model obtained is smoothed too much everywhere in the compu-547 tational domain. In Figure A4, an extreme case without data misfit minimization is considered while 548 keeping the cross-gradient term only in the total misfit cost function. We can observe that the data 549 distribution is reaching values closer to the real gravity data with a pronounced smoothing around the 550 highest anomaly values. 551

In summary, these different tests suggest that more physical inverted physical models can be obtained during the inversion process by introducing a Nafe-Drake prior model as a starting model or into the damping model term, or both, and by applying simultaneously the cross-gradient term in order to distribute physically the density variations at depth, as can be seen in 8d-e. The simultaneous min-

- imization of the gravity data misfit, the model damping regularization term and the cross-gradient is
- necessary. Now, in the next section, we show how the different terms of the cost function are behaving
- $_{\rm 558}$   $\,$  when optimal  $\lambda$  and  $\alpha$  are chosen.



**Figure A1.** (Top) PYROPE and OROGEN seismic transects, and permanent seismic stations (Chevrot et al. 2018). The triangles represent the stations of the PYROPE (blue) and OROGEN seismic transects (purple). The thick black lines represent the ECORS-Pyrenees and ECORS-Arzacq deep seismic sounding profiles, located in the Central and Western Pyrenees. (Bottom) BGI gridded Bouguer anomaly data at 2 mn arc resolution in Southwest France and North Spain. Figure extracted from Chevrot et al. (2018)



**Figure A2.** Observed and inverted gravity data with (1) or without (0) starting model, with or without model damping regularization, with or without cross-gradient constraint.



**Figure A3.** Results of inversions without any cross-gradient regularization (a to e) according to cases 1, 2 and 3. **Case 1 :** Inverted anomalies (a) and effective densities (b) are obtained without damping on the model ( $\lambda = 0$ ), without starting model and without cross-gradient ( $\alpha = 0$ ). Solutions are locate close to the surface. In Figure (c), a starting model is introduced : anomalies appear close to the surface and at depth. **Case 2 :** In Figures (d) and (e), a damping regularization is applied on the model ( $\lambda \neq 0$ ) with a starting model as in figure (c) : similar anomalies appear close to the surface and at depth when compared to figure (c) but with slightly smaller values close to the surface. **Case 3 :** In figure (f), only cross-gradient regularization is applied ( $\alpha \neq 0$ ), without imposing a starting model and without model damping ( $\lambda = 0$ ) : the solution is not physical with too much smoothing at depth.



Figure A4. Gravity data and models obtained along the seismic profile in an extreme case after minimization of the cost function involving the cross-gradient function alone (no data misfit and no damping on the model, i.e  $\lambda = 0$ , are considered) for the 2.5D case. (a-Top) Representation of the observed, prior and inverted Bouguer gravity data. (b-Middle) Data misfit between observed data and inverted data obtained after reaching a zero cross-gradient between density anomalies and  $V_p$  seismic velocities. (c-Bottom) Inverted densities respecting the zero cross-gradient condition. Too smooth models are recovered in this specific case.



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**Figure A5.** Collisional model proposed in the western Pyrennees for the Eocene to present day period by Lescoutre & Manatschal (2020), and coherent to the one proposed by Gómez-Romeu et al. (2019). Figure (A) : Southwest-northeast cross sections A and B passing through eastern and western Mauleon basin (chapter III, p. 121 of Lescoutre (2019)). Figure (B) : Cross section D passing through Eastern Mauleon (figure III-4, chapter III, p. 131 in Lescoutre (2019)) is very similar to our imaged A-A' section shown in Figure 14.