

Structure-coupled 3-D imaging of magnetotelluric and wide-angle seismic reflection/refraction data with interfaces

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Abstract

Magnetotelluric (MT) and wide-angle seismic reflection/refraction surveys play a fundamental role in understanding the crustal rheology and lithospheric structure of the Earth. In recent years, the integration of the two methods in order to improve the robustness of the inversion has started to gain attention. We present a new approach for joint 3-D inversion of MT and wide-angle seismic reflection/refraction data to accurately determine crustal structures and Moho depth. Based on H- κ stacking of teleseismic receiver functions (RFs), we estimate an initial reference Moho. This is used as input for the subsequent MT/seismic joint inversion, where the Moho interface is updated and crustal structures are added to the model. During the joint inversion process, structural similarity is facilitated through the cross-gradient constraint. Synthetic model tests show an improvement of the inversion results over separate inversions. In particular, the tests based on two geologically realistic models demonstrate that the crustal structure and even the trade-off between velocity and Moho interface can be sufficiently resolved by combined MT and seismic datasets when using the estimates from analysis of RFs. These results show that the new method can provide useful constraints on crustal structures including their geophysical properties and discontinuities.

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2 **wide-angle seismic reflection/refraction data with interfaces**

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10 **Key Points:**

- 11 • A new coupled algorithm is developed for 3-D imaging of magnetotelluric and wide-
12 angle seismic reflection/refraction data
- 13 • Two strategies are presented to mitigate the problem of accurately determining crustal
14 structures and Moho interface simultaneously
- 15 • The inclusion of teleseismic receiver functions is proved to be effective in the new
16 algorithm
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18 **Abstract**

19 Magnetotelluric (MT) and wide-angle seismic reflection/refraction surveys play a
20 fundamental role in understanding the crustal rheology and lithospheric structure of the Earth.
21 In recent years, the integration of the two methods in order to improve the robustness of the
22 inversion has started to gain attention. We present a new approach for joint 3-D inversion of
23 MT and wide-angle seismic reflection/refraction data to accurately determine crustal
24 structures and Moho depth. Based on H- κ stacking of teleseismic receiver functions (RFs),
25 we estimate an initial reference Moho. This is used as input for the subsequent MT/seismic
26 joint inversion, where the Moho interface is updated and crustal structures are added to the
27 model. During the joint inversion process, structural similarity is facilitated through the cross-
28 gradient constraint. Synthetic model tests show an improvement of the inversion results over
29 separate inversions. In particular, the tests based on two geologically realistic models
30 demonstrate that the crustal structure and even the trade-off between velocity and Moho
31 interface can be sufficiently resolved by combined MT and seismic datasets when using the
32 estimates from analysis of RFs. These results show that the new method can provide useful
33 constraints on crustal structures including their geophysical properties and discontinuities.

34 **1 Introduction**

35 The magnetotelluric (MT) method provides crucial information on the conductivity of the
36 subsurface of the Earth determined by the presence of interconnected fluids and partial melt
37 and is widely used to image the lithosphere-asthenosphere system [e.g., [Jones, 1999](#);
38 [Unsworth, 2010](#); [Lin et al. 2017](#)]. In contrast, wide-angle seismic surveys image gradual
39 changes in velocity and distinct geological features such as interfaces between layers and
40 unconformities in the crust using controlled or artificial sources [[Rawlinson et al., 2001](#)].
41 Based on such measurements, both layer velocity and interface geometry can be retrieved
42 from reflection and/or refraction travel times using tomographic approaches [[Zelt et al., 1992](#);
43 [Rawlinson et al., 2010](#); [Karplus, et al. 2011](#)].

44 The combination of multiple geophysical data types can help reduce the non-uniqueness of
45 inversion results [e.g., [Moorkamp, 2017](#)]. For example, seismic methods generally have
46 reliable vertical resolution on horizontal or dipping planar layers. They can effectively
47 compensate the diffusive nature of electromagnetic fields that leads to decreased vertical
48 resolution in the deeper earth and generally smooth models [[Chave and Jones, 2012](#)].
49 Conversely, blind areas of seismic refraction may exist in some cases but can be improved by
50 MT surveys [[Stanley et al., 1990](#); [Bennington et al., 2015](#)]. Another benefit of combining MT

51 and wide-angle seismic data is that they sense structures on similar spatial scales, and
52 therefore can be effectively compared or coupled.

53 In recent times, a number of studies have been performed utilizing joint inversion of MT
54 and seismic traveltime data [e.g., [Heincke et al., 2006](#); [Gallardo, 2007](#); [2012](#); [Hu et al., 2009](#);
55 [Moorkamp et al., 2011](#); [Peng et al., 2013](#)]. In terms of coupling approach, these studies can
56 be classified into two main categories: direct petrophysical parameter coupling [e.g.,
57 [Colombo and Stefano, 2007](#); [Heincke et al., 2017](#)] and structural coupling [e.g., [Haber and](#)
58 [Oldenburg, 1997](#); [Gallardo and Meju, 2003](#)]. The former approach focuses on explicit
59 functional relationships between electrical resistivity and seismic velocity. These can be
60 estimated from empirical laws based on rock physics such as Archie and Wyllie equations
61 [[Archie, 1942](#); [Wyllie et al., 1956](#)], derived from borehole data and porosity estimations [e.g.,
62 [Jegen et al. 2009](#); [Berryman et al., 2002](#)], or calculated from composition and temperature of
63 the mantle [[Afonso et al. 2013](#)]. However, these methods largely depend on a-priori
64 petrophysical relationships, and if the relationships are estimated incorrectly, it is likely to
65 lead to artifacts in the joint inversion results [[Moorkamp et al. 2011](#)].

66 Structural coupling approaches were first proposed to measure structural similarity using
67 model curvature to enhance common boundaries [[Zhang and Morgan; 1997](#); [Haber and](#)
68 [Oldenburg, 1997](#)]. [Gallardo and Meju \[2003\]](#) introduced the cross-gradient method to
69 consider direction-dependent constraints on different models. This direction-based approach
70 is widely applicable and has been adapted to different geophysical data types [[Gallardo and](#)
71 [Meju, 2011](#); [Linde et al., 2006](#); [Fregoso and Gallardo, 2009](#); [Doetsch et al., 2010](#); [Moorkamp](#)
72 [et al., 2016](#)], since it provides a generalized methodology for evaluating structural similarity
73 between diverse multidimensional models.

74 In wide-angle seismic surveys, crustal structure is commonly represented by a series of
75 sub-horizontal layers separated by continuous interfaces. In comparison with traditional
76 refraction interpretation, using both refracted and reflected phases to image seismic structure
77 offers potentially better resolution [[Rawlinson et al., 2001](#); [Rawlinson and Urvoy, 2006](#)].
78 However, although a few recent studies have taken these reflection travel times into
79 consideration by jointly inverting multiple geophysical data sets with application to marine
80 subsurface integrated imaging [e.g., [Gallardo et al., 2012](#)], examples of hybrid 3-D joint
81 inversion frameworks that determine interface depths and physical properties simultaneously
82 are harder to find. One issue with inverting reflection travel time is the difficulty to include
83 data that involve seismic discontinuities, such as Moho reflections. Another problem is that
84 there is a trade-off between Moho boundary location and crustal velocity which can be

85 largely attributed to inadequate path coverage near the Moho interface [Rawlinson et al.,
86 2010].

87 In this paper, we introduce a 3-D cross-gradient joint inversion algorithm that combines
88 MT data with seismic reflection and refraction travel times. For the seismic tomography part
89 of the algorithm, we consider a layered medium in a discontinuous velocity model intersected
90 by an undulating Moho interface, allowing both seismic reflection and refraction phases to be
91 tracked. Additional constraints from teleseismic RFs are also included in the new framework
92 in order to overcome the limitation of accurately determining crustal structures and Moho
93 interface simultaneously under geologically realistic conditions.

94 **2 Forward Modeling Algorithms**

95 **2.1. Forward Modeling in MT Method**

96 We use a 3-D staggered-grid finite difference method (SFD) as the forward algorithm for
97 electromagnetic (EM) modeling [Tan et al., 2003]. Similar to previous work for computing
98 the MT response of 3-D Earth models [Mackie et al., 1993], the algorithm is based on the
99 integral forms of Maxwell's equations given by:

$$100 \quad \oint \mathbf{H} \cdot d\mathbf{l} = \iint \mathbf{J} \cdot d\mathbf{S} = \iint \sigma \mathbf{E} \cdot d\mathbf{S} \quad (1)$$

$$101 \quad \oint \mathbf{E} \cdot d\mathbf{l} = \iint i\mu\omega \mathbf{H} \cdot d\mathbf{S}, \quad (2)$$

102 where \mathbf{J} is current density, σ is conductivity, ω is angular frequency, $d\mathbf{l}$ is the contour of
103 integral closure, and $d\mathbf{S}$ is the area closed by the contour.

104 After spatial discretization on a staggered-grid with appropriate boundary conditions,
105 integral equations (1) and (2) can be expressed as a complex system of large-scale linear
106 equations. In this scheme [Tan et al. 2003], the linear equations are solved by using a
107 stabilized Bi-conjugate gradient method and generate high-precision electric or magnetic
108 field component efficiently. The complex impedance tensor (Z_{xx} , Z_{xy} , Z_{yx} , and Z_{yy}) can be
109 computed from the electromagnetic fields along two orthogonal directions in four equations
110 [e.g. Egbert and Kelbert, 2012].

111 Moreover, a parallel scheme was developed by adding Message Passing Interface (MPI)
112 approach running on computer clusters in order to reduce computational time [Tan et al.,
113 2006]. As the 3-D joint inversion requires a significant amount of computation, this parallel
114 3-D MT forward modeling scheme is particularly suited for it.

115 **2.2. Traveltime Computation in Wide-angle Seismic Reflection/refraction Method**

116 We use a multi-stage Fast Marching Method (FMM) [Rawlinson and Sambridge, 2005] as
 117 the forward method to compute theoretical travel times of seismic waves in a known 3-D
 118 velocity model volume, given hypocenter locations and receiving stations on the Earth
 119 surface. FMM is a grid based eikonal solver that can implicitly track the evolution of
 120 wavefronts for calculating reflection and refraction phases in layered media [Rawlinson and
 121 Sambridge, 2004; de Kool et al, 2006].

122 For a seismic P-wave in an isotropic elastic medium, the eikonal equation can be written
 123 as:

$$124 \quad |\nabla T| = \frac{1}{\mathbf{v}}, \quad (3)$$

125 where ∇ represents gradient operator, $T=T(x)$ is a time function (the traveltime) which
 126 describes surfaces of constant phase (wavefronts) when T is constant, and \mathbf{v} is the seismic
 127 wave velocity as a function of the position at a spatial point. This equation describes the time
 128 of arrival of the fastest wave front at a given position.

129 Recently, an upwind scheme [de Kool et al, 2006] has been implemented for predicting
 130 multi-arrivals. One advantage of the practical grid-based method is that the propagation grid
 131 is defined separately from the inversion grid by specifying discrete sampling of velocity
 132 fields and implicit interface boundaries. Because it has no direct relationship with the
 133 inversion grid, we can consider both the calculation accuracy of forward modeling and the
 134 scale of the inversion grid. Also, adding interface nodes does not significantly increase the
 135 complexity of the inversion grid, which is another benefit for the joint inversion framework.

136 For our inversion we use the FMM algorithm with the upwind scheme implemented in the
 137 FMTOMO package developed by Rawlinson and Sambridge [2005]. Tests with a variety of
 138 velocity structures show that it is both computationally efficient and robust and thus
 139 preferable as a forward solver for reflection and refraction data for the joint inversion.

140 **3 Inversion Algorithms**

141 In addition to well-developed separate forward modeling algorithms, a flexible 3-D joint
 142 inversion framework needs large-scale optimization inversion schemes and a coupling
 143 approach.

144 In our implementation, the resistivity model and velocity model parameters are updated in
 145 an exchanging pattern that is similar to the approach by Um et al. [2015]. In addition, we also
 146 consider the determination of an initial Moho interface (\mathbf{H}) and its adjustment during the

147 velocity model updates in the algorithm.

148 The framework (Figure 1) is composed of two main modules (MT inversion module &
 149 seismic inversion module). Neither of them is independent of each other as they are linked by
 150 cross-gradient coupling at each iteration of a loop. Taking the MT inversion module, for
 151 example, we carry out the MT inversion first when the joint inversion starts. The parallel
 152 SFD forward solver as shown below is used to calculate theoretical electromagnetic
 153 responses from an initial resistivity model \mathbf{m}_ρ^0 . Then, in a cross-gradient coupling module, we
 154 calculate the cross-gradient values ($\boldsymbol{\tau}$) and its Jacobian matrix (\mathbf{B}) between the initial
 155 resistivity model \mathbf{m}_ρ^0 and the velocity model \mathbf{m}_s^0 , respectively. The first updated resistivity
 156 model \mathbf{m}_ρ^1 is generated by the model update expression of the data-space method as presented
 157 in Eq. (12). After that, we need to calculate the misfit (RMS) between the observed data and
 158 the synthetic responses and estimate if the value is lower than the desired level of misfit. We
 159 then perform similar computations for the seismic part of the inversion. The iteration loop
 160 will not end until both MT RMS and seismic RMS satisfy the requirement of error tolerances
 161 or reach the maximum number of iterations.

162 In the following section, we first introduce the MT and tomographic inversion schemes,
 163 and then present the model coupling approach and how the two methods are combined. We
 164 then discuss our strategy to estimate crustal thickness within the inversion and how it impacts
 165 on the tomographic results.

166 3.1. MT Inversion Scheme

167 The classical Occam's inversion seeks models fitting the data while at the same time
 168 having the "smoothest" structure [Constable et al. 1987]. The inversion uses a self-adaptive
 169 regularization scheme, which is affected little by the initial model and has a stable
 170 convergence [de Groot-Hedlin and Constable, 1990], thus it is an ideal algorithm to solve MT
 171 inverse problems. The minimization of the objective function is achieved by finding
 172 stationary points of the equation:

$$173 \quad U(\mathbf{m}_\rho, \lambda) = \left\| \mathbf{m}_\rho - \mathbf{m}_\rho^0 \right\|_{\mathbf{C}_m^{-1}}^2 + \lambda^{-1} \left(\left\| \mathbf{d}_{\text{obs}} - f(\mathbf{m}_\rho) \right\|_{\mathbf{C}_d^{-1}}^2 - \xi \right), \quad (4)$$

174 where \mathbf{m}_ρ is the vector of resistivity model parameters, \mathbf{m}_ρ^0 is the vector of priori model
 175 parameters, \mathbf{C}_m is the model covariance matrix, \mathbf{d}_{obs} is the vector of observed data, $f(\mathbf{m}_\rho)$
 176 is the model response, \mathbf{C}_d is the data covariance matrix, ξ is the desired level of misfit, and
 177 λ^{-1} is a Lagrange multiplier.

178 To find a new model we linearize the above objective function U , and obtain a series of
 179 iterative solutions:

$$180 \quad \mathbf{m}_\rho^{k+1}(\lambda) = (\lambda \mathbf{C}_m^{-1} + \mathbf{J}_k^T \mathbf{C}_d^{-1} \mathbf{J}_k)^{-1} \mathbf{J}_k^T \mathbf{C}_d^{-1} \mathbf{X}_k + \mathbf{m}_\rho^0, \quad (5)$$

181 where \mathbf{J}_k is the corresponding Jacobian matrix, $\mathbf{X}_k = \mathbf{d}_{obs} - f(\mathbf{m}_\rho^k) + \mathbf{J}_k(\mathbf{m}_\rho^k - \mathbf{m}_\rho^0)$, and the
 182 inverse matrix $\mathbf{\Lambda}_k^{-1} = (\lambda \mathbf{C}_m^{-1} + \mathbf{J}_k^T \mathbf{C}_d^{-1} \mathbf{J}_k)^{-1}$ is a $M \times M$ positive semi-definite symmetric matrix
 183 in model space, where M is the number of model parameters.

184 [Siripunvaraporn et al. \[2005\]](#) reformulate Occam's inversion scheme into data-space in
 185 order to avoid the computational cost of inverting a $M \times M$ matrix. They transform the above
 186 iterative Eq. (5) mathematically into a new one that contains a $N \times N$ system of linear normal
 187 equations:

$$188 \quad \mathbf{m}_\rho^{k+1}(\lambda) = \mathbf{C}_m \mathbf{J}_k^T (\lambda \mathbf{C}_d + \mathbf{J}_k \mathbf{C}_m \mathbf{J}_k^T)^{-1} \mathbf{X}_k + \mathbf{m}_\rho^0. \quad (6)$$

189 Here N is the number of independent data, which for many geophysical surveys is orders
 190 of magnitude smaller than the number of model parameters M .

191 The data-space method is similar to Occam's inversion approach as the model iterations in
 192 data-space also follow the principle of minimizing a penalty function with a series of
 193 Lagrange multipliers λ . The data-space algorithm has been shown to be efficient in 3-D MT
 194 inversion in terms of reducing the matrix dimensions since the number of independent data N
 195 in realistic models is normally much less than the number of model parameters M , which
 196 results in significant savings of both memory and CPU time [[Siripunvaraporn and Egbert,](#)
 197 [2009](#)].

198 Another advantage of the data-space method is that a generalized model covariance \mathbf{C}_m is
 199 directly calculated, thus it avoids solving the inverse of the full matrix \mathbf{C}_m , which can result
 200 in large computational costs. Note that for model space inversion approaches [[Constable et al.,](#)
 201 [1987; deGroot-Hedlin and Constable, 1990](#)], it is common to utilize a sparse model
 202 roughness operator in terms of a "roughness penalty" instead of directly using the model
 203 covariance \mathbf{C}_m . [Siripunvaraporn and Egbert \[2000\]](#) discuss the differences between them in
 204 detail and how to deal with the \mathbf{C}_m in the data-space algorithm.

205 **3.2. Tomographic Inversion Scheme**

206 We use a nonlinear subspace inversion approach to implement the tomographic inversion
 207 procedure. Similar to the MT inversion scheme, the inverse problem can be solved by
 208 specifying an objective function to adjust the model parameter values (i.e., velocity \mathbf{m}_s and
 209 interface depth \mathbf{H}) and try to satisfy the data observations (source-receiver travel times),
 210 subject to imposed regularization constraints. The scheme is implemented by a least squares
 211 approximation to a multi-dimensional subspace of model space using the iterative subspace
 212 method [[Kennett et al., 1988; Sambridge, 1990](#)]. The model update is composed of a series of

213 base vectors in terms of the steepest ascent vector in model space and the perturbation of
 214 model is finally written as:

$$215 \quad \delta \mathbf{m}_{sh} = -\mathbf{A}[\mathbf{A}^T (\mathbf{G}^T \mathbf{C}_d^{-1} \mathbf{G} + \varepsilon \mathbf{C}_m^{-1}) \mathbf{A}]^{-1} \mathbf{A}^T \boldsymbol{\gamma}, \quad (7)$$

216 where, \mathbf{A} is a projection matrix $[\mathbf{a}^j]$; $\{\mathbf{a}^j\}$ is the spanning set of basis vectors; $\boldsymbol{\gamma}$ is the gradient
 217 vector; \mathbf{G} is the Jacobian matrix of partial derivatives; the variables \mathbf{A} , $\boldsymbol{\gamma}$ and \mathbf{G} are updated
 218 constantly in successive iteration. Here the vector $\delta \mathbf{m}_{sh}$ includes two classes of model
 219 parameters: the velocities and the depths of the interface vertices. For the derivation and
 220 simplification of the equation, see [Rawlinson et al. \[2001\]](#).

221 Once the projection matrix \mathbf{A} has been computed and orthonormalized, the model update is
 222 obtained by the inversion of a relatively small matrix. The subspace inversion method is
 223 stable and efficient for large underdetermined inverse problems, and together with FMM,
 224 forms the basis of a fast and robust tomographic imaging scheme. Singular value
 225 decomposition (SVD) is used to identify and remove unnecessary basis vectors if \mathbf{A} does not
 226 completely span all dimensions. Usually the value of the dimension size of \mathbf{A} is small, for
 227 example, the dimension size used by [Rawlinson and Urvoy \[2006\]](#) is less than 20 when they
 228 implemented inversion of observed traveltimes data from Tasmania, Australia. In this paper,
 229 the dimension of the subspace used in the tomographic inversion was set to 18 in that it offers
 230 a suitable compromise between the reduction of the misfit function and the computational
 231 burden.

232 **3.3. Joint Inversion Algorithm**

233 **3.3.1. Coupling Approach**

234 We enforce structural similarity between resistivity and P-wave velocity through the cross-
 235 gradient approach [[Gallardo and Meju, 2003](#)]. The cross-gradient function is defined as:

$$236 \quad \boldsymbol{\tau}(x, y, z) = \nabla \mathbf{m}_\rho(x, y, z) \times \nabla \mathbf{m}_s(x, y, z), \quad (8)$$

237 where \mathbf{m}_ρ and \mathbf{m}_s represent the electrical resistivity model vector and the seismic P-wave
 238 velocity vector, respectively. Note that $\boldsymbol{\tau}(x, y, z)$ is a spatial vector in any grid that has three
 239 components (τ^x , τ^y , and τ^z) along the coordinate axis in x, y and z direction, respectively.
 240 Here, the resistivity (ρ) and velocity (v) are transformed into $\log \rho$ and $1/v$ when calculating
 241 cross-gradient values, to ensure that the variation in regions of high and low value of the
 242 model parameters will have a similar scale and can exert identical importance on the
 243 structural similarity.

244 In order to generate more precise results compared with our previous forward difference

245 scheme [Peng et al., 2013], we use a central difference scheme here to discretize the cross-
246 gradient in a 3-D subsurface medium (Figure 2).

247 The joint inversion algorithm requires the Jacobian matrix \mathbf{B} associated with the cross-
248 gradient function with regards to the model parameters. In our approach, the cross-gradient
249 function for the current iteration is approximately linearized by a first-order Taylor expansion
250 around their a-priori models [Gallardo and Meju, 2004]. Note that the matrix \mathbf{B} is
251 decomposed into three orthogonal components \mathbf{B}^x , \mathbf{B}^y , and \mathbf{B}^z . Each of the components is a
252 sparse matrix in which every row has 10 nonzero elements in the central mesh. In addition,
253 there are even less than 10 nonzero elements on the boundaries of the mesh depending on
254 which region of the grid we deal with, i.e., the boundary surface, the edges or the vertices. To
255 avoid large-scale matrix calculation, we use the compressed sparse row (CSR) format to store
256 elements of \mathbf{B} and utilize the efficient algorithms to manipulate sparse matrices implemented
257 in the SPARSEKIT package [Saad, 1990].

258 3.3.2. Objective Function

259 In addition to the data misfit terms and the regularisation terms for separate inversion, the
260 cross-gradient term for structural coupling [Gallardo and Meju, 2003] is added in the
261 objective function to enforce structural similarity between resistivity and velocity. The
262 framework of the joint inversion algorithm can be divided into two connected parts as shown
263 in Figure 1: the MT inversion scheme and the seismic tomographic inversion scheme. With
264 the structural coupling constraint the respective objective functions Ψ are then defined as:

$$265 \Psi_{\text{MT}}(\mathbf{m}_p, \lambda) = \|\mathbf{m}_p - \mathbf{m}_p^0\|_{\mathbf{C}_m^{-1}}^2 + \lambda^{-1} \left[\|\mathbf{d}_p - f(\mathbf{m}_p)\|_{\mathbf{C}_d^{-1}}^2 \right. \\ \left. + \mu_p \|\boldsymbol{\tau}(\mathbf{m}_p, \tilde{\mathbf{m}}_s) - \boldsymbol{\tau}(\mathbf{m}_p^0, \mathbf{m}_s^0)\|_{\mathbf{C}_\tau^{-1}}^2 - \xi \right], \quad (9)$$

$$266 \Psi_{\text{Seis}}(\mathbf{m}_s, \mathbf{H}) = \|\mathbf{m}_s - \mathbf{m}_s^0\|_{\mathbf{C}_m^{-1}}^2 + \varepsilon^{-1} \left[\|\mathbf{d}_s - g(\mathbf{m}_s)\|_{\mathbf{C}_d^{-1}}^2 \right. \\ \left. + \mu_s \|\boldsymbol{\tau}(\tilde{\mathbf{m}}_p, \mathbf{m}_s) - \boldsymbol{\tau}(\mathbf{m}_p^0, \mathbf{m}_s^0)\|_{\mathbf{C}_\tau^{-1}}^2 \right], \quad (10)$$

267 where \mathbf{m}_p (logarithm of resistivity) and \mathbf{m}_s are the vector of current model parameters, $\tilde{\mathbf{m}}_p$,
268 $\tilde{\mathbf{m}}_s$ are the vector of the model parameters updated during the latest MT and seismic
269 tomographic inversion respectively. $f(\mathbf{m}_p)$, $g(\mathbf{m}_s)$ denote the model response from the
270 forward calculation for MT and the seismic method respectively, \mathbf{d}_p , \mathbf{d}_s are the vector of
271 MT and seismic observed data, $\boldsymbol{\tau}(\cdot)$ is the cross-gradient operator, \mathbf{C}_τ denotes the cross-

272 gradient covariance matrix that is an identity matrix, ε , λ are the regularization weighting
 273 factors, and μ_p , μ_s are the weighting factors of the cross-gradient terms.

274 In our joint inversion algorithm, the updated models are not used in integrated objective
 275 function. Instead the models are mutually constrained by the results of a previous iteration
 276 from the other method. As described above, we use the data-space method and the subspace
 277 method as the optimization algorithm respectively. For the MT module, we solve the inverse
 278 problem in the sense of [Siripunvaraporn et al. \[2005\]](#) and derive a new iterative formula to
 279 minimize the objective function of Ψ_{MT} in Eq. (9) which includes the coupling term. The
 280 expression (see Appendix A) for a series of model updates from an initial model is:

$$281 \quad \mathbf{m}_p^{k+1}(\lambda) = \mathbf{C}_m \mathbf{J}_k^T \Gamma_k^{-1} \mathbf{X}_k - \mu_p \Lambda_k^{-1} \left[(\mathbf{B}_p^k)^T \mathbf{C}_\tau^{-1} \mathbf{B}_p^k (\mathbf{m}_p^k - \mathbf{m}_p^0) \right] + \mathbf{m}_p^0, \quad (11)$$

282 where $\Gamma_k^{-1} = (\lambda \mathbf{C}_d + \mathbf{J}_k \mathbf{C}_m \mathbf{J}_k^T)^{-1}$, and $\Lambda_k^{-1} = \frac{1}{\lambda} (\mathbf{I} - \mathbf{C}_m \mathbf{J}_k^T \Gamma_k^{-1} \mathbf{J}_k) \mathbf{C}_m$.

283 Here, $\mathbf{B}_p = \mathbf{B}_p^x(\tilde{\mathbf{m}}_s) + \mathbf{B}_p^y(\tilde{\mathbf{m}}_s) + \mathbf{B}_p^z(\tilde{\mathbf{m}}_s)$ is the Jacobian matrix of the cross-gradient with
 284 respect to the current resistivity model \mathbf{m}_p , but only determined by the velocity model $\tilde{\mathbf{m}}_s$
 285 that is updated during the latest seismic inversion. The definition of the vector \mathbf{X}_k in Eq. (11)
 286 is identical to that given by Eq. (5). In fact, compared with the separate MT inversion in Eq.
 287 (6), the second term in Eq. (11) is an added cross-gradient constraint that can make the
 288 structural features of current resistivity model similar to the previous seismic model.

289 To adapt the subspace method [[Kennett et al 1988](#), [Sambridge, 1990](#)] to our joint inversion
 290 optimisation problem for the seismic module, we rewrite the gradient vector and Hessian
 291 matrix in a new form by evaluating derivatives of objective function Ψ_{Seis} in Eq. (10). The
 292 solution is given by the following expressions (see Appendix B for more detail):

$$293 \quad \delta \mathbf{m}_s = -\mathbf{A} [\mathbf{A}^T (\mathbf{G}^T \mathbf{C}_d^{-1} \mathbf{G} + \varepsilon \mathbf{C}_m^{-1} + \mu_s \mathbf{B}_s^T \mathbf{C}_\tau^{-1} \mathbf{B}_s) \mathbf{A}]^{-1} \mathbf{A}^T \boldsymbol{\gamma}, \quad (12)$$

$$294 \quad \boldsymbol{\gamma} = \mathbf{G}^T \mathbf{C}_d^{-1} [\mathbf{d}_s - g(\mathbf{m}_s)] + (\varepsilon \mathbf{C}_m^{-1} + \mu_s \mathbf{B}_s^T \mathbf{C}_\tau^{-1} \mathbf{B}_s) \cdot (\mathbf{m}_s^0 - \mathbf{m}_s), \quad (13)$$

295 where the Jacobian matrix of the cross-gradient \mathbf{B}_s is also decomposed into three components
 296 and only determined by the resistivity model $\tilde{\mathbf{m}}_p$ that is updated during the latest MT
 297 inversion.

298 This form of objective function we adopt here is slightly different from the approach
 299 introduced by [Gallardo and Meju \[2003\]](#). Their approach minimizes the objective function
 300 including the data misfit term and the regularisation term above but requires the cross-
 301 gradient term to be equal to zero, and thereby searches exact structural resemblance.

302 Although such an approach provides the benefit of fully enforcing the sought structural
303 similarity, it poses some limitations on large-scale 3-D joint inverse problems [Meju and
304 Gallardo, 2016]. Instead our approach only seeks partial resemblance, as the cross-gradient
305 term can deviate from zero. In addition, updating the model in an alternating manner can, in
306 theory, lead to less strict coupling between the methods. However, such mutually constrained
307 inversion algorithms have been shown to be effective in previous studies [e.g., Um et al.,
308 2014, Heincke et al., 2017] and offer high flexibility to integrate new methods.

309 **3.3.3. Inverting for Seismic Layer Interfaces**

310 First experiments with our coupled MT/seismic inversion show that it is important to
311 consider the effect of variations in reflector positions in the seismic tomography. The
312 inversion therefore also contains a module to update the position of chosen reflective
313 interfaces.

314 The inclusion of interfaces can potentially increase the non-uniqueness of the solution
315 because the amount of model parameters is larger if we invert for physical properties and
316 depths of the interface vertices simultaneously. Also, we found that in geologically realistic
317 situations the estimates of crustal velocity and Moho interface provided by separate
318 tomographic inversions are likely to be inaccurate because of the trade-off between Moho
319 boundary location and crustal velocity. This can be largely attributed to inadequate path
320 coverage near the Moho interface. We propose two strategies in order to overcome such
321 limitations.

322 The first strategy is to invert for resistivities and velocities with fixed interfaces determined
323 by prior information. We can acquire relatively accurate information on the Moho interface
324 and one-dimensional layered velocity model before starting a 3D inversion. This can be done
325 by 1-D joint inversion of RFs and surface wave dispersion data [e.g., Moorkamp et al., 2010;
326 Peng et al., 2012]. With a good constraint on the location of the Moho interface or the
327 layering of the subsurface, an approach to jointly invert crustal structure with a fixed Moho
328 interface can be feasible. However, the success of such a strategy largely depends on the
329 initial model and the accuracy of the fixed Moho interface and thus is hard to judge.

330 Another choice is to update the location of interfaces while resistivities and velocities are
331 jointly estimated. The advantage is that this strategy does not need rigorous requirement on
332 the initial Moho boundary that may be not very close to the true Moho. This is therefore our
333 preferred approach.

334 As RFs are sensitive to velocity discontinuities, they are considered to be an ideal tool to
335 recover the position of the Moho interface. A grid search method [Zhu and Kanamori, 2000],

336 H- κ stacking, is widely used to estimate crustal thickness H and V_p/V_s ratio (κ). Such an
 337 “inaccurate” Moho interface can be estimated from RFs and used as an initial reference Moho
 338 for the 3-D joint inversion.

339 However, if there is a 0.2 km/s deviation on average P wave velocity (\bar{V}_p) in the process of
 340 H- κ stacking, it can give rise to an average error of 1.8 km in estimating Moho depth [Zhu et
 341 al., 2006]. Thus, in some study areas with little priori information on \bar{V}_p , the method can lead
 342 to controversial results [Wölbern and Rümper, 2017]. In this paper, we present an effective
 343 way of mitigating this problem by using an updated crustal model to calculate more accurate
 344 \bar{V}_p from the results of seismic refraction/reflection tomography. We use interface nodes (j)
 345 corresponding to different \bar{V}_p because the layer velocity V_p^i is different beneath each
 346 broadband seismic station (j). This \bar{V}_p^j can be easily obtained by calculating the average
 347 velocity in the model underneath each station viz:

$$348 \quad \bar{V}_p^j \approx \frac{H}{\sum_{i=1}^{N(j)} (\Delta z / V_p^i)} \quad (\text{km/s}), \quad (14)$$

349 where H is the Moho depth, Δz is the interlayer spacing in the depth direction, and $N(j)$ is
 350 the number of layer of the crust beneath the j^{th} seismic station. At each iteration, the Moho
 351 interface is updated by H- κ stacking with the new \bar{V}_p . Then, the updated Moho interface is
 352 used as the reference interface for the seismic joint inversion during the next iteration.

353 We finally note that the rates of convergence between MT and seismic inversion can vary
 354 significantly. This was also observed by Heincke et al. [2017], and may result in abnormal
 355 coupling in the process. For example, assuming that seismic inversion converges much more
 356 slowly than MT inversion, the latter would be constrained by an incomplete velocity model
 357 when the MT inversion ends. Therefore, we adjust the cross-gradient coupling flexibly by
 358 estimating which updated model should be used in the cross-gradient module. In this paper,
 359 we only have 4 iterations in MT inversion but 12 iterations in seismic inversion, so at each
 360 iteration the joint MT inversion is constrained by renewed resistivity model whose estimated
 361 iteration is multiple of 3.

362 **4 Synthetic Examples and Discussions**

363 We now apply the method above to synthetic examples to test the joint inversion algorithm.
 364 All computations were performed on the Alice2 cluster at the University of Leicester. Each
 365 compute node has a pair of 14-core Intel Xeon Skylake CPUs running at 2.6GHz, and 128GB
 366 of RAM. For the first two synthetic examples, the subsurface region for joint inversion is

367 discretized with a $20 \times 20 \times 20$ mesh yielding 8,000 equally-sized cells. Cell sizes in the interior
 368 of the mesh are $5 \times 5 \times 4$ km.

369 The wide-angle synthetic dataset comprises more than 3800 crustal reflection (PmP) and
 370 refraction (Pg & Pn) travel times generated by 9 active sources and recorded by 144 receivers
 371 evenly distributed on a grid at the surface (Figure S1).

372 We place 36 MT sites on the surface and calculate the complex impedance tensor (Z_{xx} ,
 373 Z_{xy} , Z_{yx} and Z_{yy}) for five frequencies (10, 1, 0.1, 0.01 and 0.001 Hz). Gaussian noise with 2%
 374 is added to the synthetic MT data and a standard deviation of 5 ms to the synthetic travel
 375 times. The data variance is assumed to be 2% of $|Z_{xy} Z_{yx}|^{1/2}$ for MT inversion and 5 ms for
 376 seismic inversion.

377 **4.1. Example I: A Simple Model Inverted with Fixed Moho Interface**

378 As a first test, we design a simple model where the resistivity and velocity of anomalies
 379 have exactly similar spatial structure features and proportional parameter values. We apply
 380 the workflow to examine how the structure-coupled 3-D joint algorithm behaves when fixing
 381 the Moho interface.

382 The model consists of two prisms within a given background (a $100 \Omega \cdot \text{m}$ half-space
 383 background for MT model and a layered background for seismic model with velocities
 384 ranging from 5.25 km/s to 8.15 km/s), and is very similar to the test model of Moorkamp et al.
 385 [2011]. Also, for the seismic model, a fixed undulated Moho boundary is defined here in
 386 order to track multiple reflection phases in the layered media. Figure 3 displays a plot of the
 387 true model used to generate the theoretical synthetic dataset.

388 The joint inversion starts from a simple background without two prisms: a $100 \Omega \cdot \text{m}$ half
 389 space and a layered velocity model (the same as the layered background for seismic model).
 390 These models were also used for the a-priori models in the joint inversion. To seek out the
 391 final optimal model, we have performed dozens of joint inversions with different cross-
 392 gradient weights. Figure 4a shows the convergence curves for the last three iterations of the
 393 joint inversion. We can see that within four iterations, the MT inversion has converged to the
 394 desired level of misfit, while the seismic inversion requires 12 iterations to achieve the target
 395 misfit. When the value of the cross-gradient weight is small (1.0~2.0), both MT and seismic
 396 data misfit change slightly due to the loose structural coupling. However, we can obtain a
 397 reasonable reduction in misfit for the last iteration when choosing somewhat larger weights
 398 (e.g., $\mu_p = 2.2 \sim 3.0$ for MT inversion and $\mu_s = 4.0 \sim 4.6$ for seismic inversion). When using very
 399 high coupling values the data misfit values strongly increase as the inversion only tries to
 400 create structurally similar models and ignores the data. These convergence curves help us to

401 find a couple of corresponding cross-gradient weights for the optimal joint inversion model
 402 (shown as asterisk in Figure 4a).

403 We evaluate the misfit between the true model and the joint inverted model when the data
 404 misfit displays little difference. This model perturbation RMS is defined as [Moorkamp et al.,
 405 2011]:

$$406 \quad \delta = \sqrt{\sum_{i=1}^M \left(\frac{\mathbf{m}_i^{true} - \mathbf{m}_i^{inv}}{\mathbf{m}_i^{true}} \right)^2}. \quad (15)$$

407 Here \mathbf{m}_i^{true} and \mathbf{m}_i^{inv} denote the model parameters in each cell for the true model and the
 408 inversion result respectively, and M is the total number of model parameters. If we choose
 409 $\mu_\rho=3.0$ and $\mu_s=4.5$ as the final cross-gradient weights we obtain $\delta_\rho=2.54$ and $\delta_s=4.28$, both
 410 of which are the minimum model perturbation RMS among all inverted models in Figure 4.
 411 In comparison, the values for the individual inversions are $\delta_\rho=2.73$ and $\delta_s=4.82$,
 412 respectively. This illustrates that the model values of the joint inversion are closer to the true
 413 values than those of the model from separate inversion.

414 The data misfit (χ) for the final joint inversion models are compared with separate
 415 inversion models varying with iteration (Figure 4b). The MT data misfit decreases from an
 416 initial value of 2.635 to 0.9996 at iteration 4. Correspondingly, the seismic misfit diminishes
 417 monotonically from 80.58 to 1.171, a value close to the noise level. We see a slower
 418 convergence rate in separate inversions, overtaken by joint inversion during the second half
 419 of the iterative process.

420 As shown in Figure 5 (a) and (c), the result of the single MT inversion differs from that of
 421 the single seismic inversion. We see that the inversion of MT data alone can recover the
 422 general shape and position of the right conductive anomaly, but the left high-resistive prism
 423 fails to be delineated in the box. The separate seismic inversion can recover the shape of the
 424 two prisms, whereas the values of the seismic velocity in the boxes cannot be fully recovered,
 425 especially at a depth of 15~20km. Compared to the separate inversions, we can see that the
 426 general shape and values of both anomalies are recovered much better in the joint inversions
 427 (Figure 5b and 5d). These jointly reconstructed resistivity and velocity models,
 428 to some extent, overcome some of the shortcomings of the separate inversions and thus
 429 improve the inversion results.

430 We also compare the computed values of the cross-gradients for MT and seismic models
 431 from the separate inversion with those for the joint inversion models (the third column in
 432 Figure 5). For separate inversion, the cross-gradient map shows zones of structural disparity
 433 especially near the boundary of anomalies. In comparison, some of the high values of cross-

434 gradients in those zones decrease obviously in the joint inversion. This observation is also
 435 confirmed by the comparison of average cross-gradients value for the final models,

$$436 \quad \bar{\tau} = \frac{1}{M} \sqrt{\sum_{i=1}^M [(\tau_i^x)^2 + (\tau_i^y)^2 + (\tau_i^z)^2]} \quad (16)$$

437 We obtain the average cross-gradients of $\bar{\tau}=4.31 \times 10^{-4}$ for the joint inversion, which is
 438 smaller than the value ($\bar{\tau}=5.32 \times 10^{-4}$) for the separate inversion. The results demonstrate that
 439 the effective cross-gradients constraint facilitate mutual structural attributes between these
 440 models.

441 **4.2. Example II: A Complex Model with Moho Perturbations**

442 We also test the joint inversion on a complex model in order to understand whether MT
 443 and seismics can help each other to recover more complex common structure. In this example,
 444 the true model consists of a plate-like resistive anomaly on top of a conductive and low-
 445 velocity block in the crust (Figure 6).

446 The a-priori models comprise a 100 $\Omega \cdot m$ half-space resistivity model and a layered seismic
 447 background model by getting rid of the anomalies. This example is a first step towards a
 448 more realistic model, as it is designed based on the typical crustal and upper mantle structure
 449 in SE Tibet. The low resistivity anomaly is based on an observed structure which has a
 450 typical bulk resistivity of 3 $\Omega \cdot m$ in most areas of southern Tibet [Unsworth et al., 2010] and
 451 has been interpreted as a partially molten layer. The velocity anomaly amplitude of the
 452 reference P wave velocity structure is set to 10% of the background based on results from
 453 joint inversion of RFs and Rayleigh wave dispersion [Sun et al., 2014]. Moho depth is usually
 454 not known a priori or difficult to determine accurately in some cases, and an inaccurate Moho
 455 position might have a negative impact on the inversion of the reflection travel times. Thus in
 456 this section, the second aim is to examine how the algorithm behaves if we are inverting for
 457 velocity parameters and interface depth simultaneously. Note that an electric Moho is not
 458 defined here because it is difficult to resolve in most localities [Jones, 2013]. Our joint
 459 inversion approach can be a contributing way to determine the exact electric Moho, but prior
 460 to the use it should be primarily established that there is an acceptable expectation of an
 461 electric Moho from the MT data.

462 Before presenting results from the test with Moho perturbations, we first conduct a test
 463 with a flat Moho at 40km depth in the starting model for the inversion. However, the results
 464 show that the crustal seismic structure is not adequately resolved by the joint inversion.
 465 Although crustal velocity at shallow depths (e.g., 0~15 km) is recovered successfully (Figure

466 7b and 7d, bottom), the velocity anomalies in the lower crust are poorly recovered. In
 467 addition, the true shape of the Moho interface seems to be difficult to recover (Figure 8c).
 468 Similar synthetic tests for this type of joint inversion (Figure S2) and the comparison to the
 469 results of crustal velocity and Moho depth with a fixed starting Moho boundary also confirm
 470 this conclusion.

471 The poor performance can be largely attributed to inadequate path coverage near the Moho
 472 interface. For separate tomographic inversion, the use of station terms or active and passive
 473 source (i.e., teleseismic events and local earthquake) datasets simultaneously can provide
 474 additional constraints on the upper-mantle velocity structure and even Moho interface
 475 [Rawlinson and Urvoy, 2006]. However, the solution not only depends on the completeness
 476 of datasets, but also suffers from the intrinsic smearing from the regularization which results
 477 in underestimating the true amplitudes of velocity structures in most tomography studies
 478 [Rawlinson et al., 2010]. Thereby, the estimates of crustal velocity and Moho interface are
 479 likely to be conservative just by separate tomographic inversion.

480 To overcome this shortcoming we simulate 36 broadband seismic stations evenly
 481 distributed on the surface (Figure 6a) and use teleseismic RFs from each station to estimate
 482 the Moho interface underneath. We found that the lateral offset of the Moho piercing point
 483 can be confined to the interface grid spacing of 12 km with an appropriate ray parameter (e.g.,
 484 <0.04 s/km). This means each broadband station can determine the crustal thickness of the
 485 grid independently using H- κ stacking technique [Zhu et al., 2006].

486 In the synthetic test, a total of 72 RFs (Figure S3) are generated with two ray parameters
 487 (0.03 s/km and 0.04 s/km) to simulate the observed data. Gaussian noise with 20% is added
 488 to the synthetic RFs directly. The initial reference Moho boundary \mathbf{H}^0 (Figure S4) can be
 489 estimated \bar{V}_p using the H- κ stacking technique based on an estimated initial V_p value of 5.4
 490 km/s. During the inversion, the interface position H gets updated and gets closer to the true
 491 Moho depth while simultaneously recalculating \bar{V}_p for each inversion iteration. Also, the
 492 updated Moho interface is used when theoretical travel times are computed during the
 493 seismic joint inversion scheme (Figure 1).

494 For the joint inversion in this example, a maximum of 18 iterations for the tomographic
 495 inversion scheme are applied to obtain solution models. The cross-gradient weights ($\mu_p=3.7$
 496 and $\mu_s=4.7$) are selected for the optimal joint inversion model. We obtain a model misfit of
 497 $\delta_p=2.73$ and $\delta_s=7.62$ for the joint inversion with the undulating Moho interface, which is
 498 smaller than those values (2.95 and 9.88) of the separate inversion.

499 Figure 7 shows the joint inversion and the separate inversion results for the realistic model

500 inverted with Moho perturbations. We can see that a significant improvement is achieved in
501 the joint inversion (especially for the velocity parameter and interface) constrained by the
502 RFs with an initially undulating Moho interface (the middle column), compared to the other
503 joint inversion case with the initial flat Moho (the left column). As both inversions are run
504 with exactly the same weights, we conclude that the additional constraints on the Moho
505 interface from RFs provide a positive contribution to the joint inversion. Although the
506 separate inversion constrained by the initial RFs (the right column in Figure 7b and Figure 7d)
507 better recovers the crustal velocity structure and Moho interface than the joint inversion with
508 a flat Moho interface, the recovery of the low-velocity anomaly in the lower crust is not
509 successful. In contrast, for the corresponding joint inversion, the modification of \bar{V}_p in the
510 joint inversion framework enables us to obtain more accurate Moho depths and thus
511 adequately resolve crustal structures by the combined datasets. Also, the image of the final
512 Moho geometry from joint inversion including the RF module (Figure 8d) is similar to the
513 true Moho interface (Figure 8a). This demonstrates that the combined datasets can resolve
514 crustal structure sufficiently and to a large degree even the trade-off between velocity and
515 Moho interface.

516 We focus much of the particular discussion on the primary interface (i.e., Moho boundary),
517 but our algorithm is applicable to a wide range of possibilities. For example, the method can
518 be well applied in a realistic multilayered crust when we are able to identify more
519 complicated phases, such as P_1P and P_2P for reflections associated with intra-crustal
520 secondary interfaces (Figure S5). In practice, the upper crustal refraction (P_g) and the Moho
521 reflection (P_mP) phases are generally easier to identify than any other arrivals (e.g. P_1 , P_2 , P_n
522 for refractions, P_1P , P_2P for reflections), but the identification of these later phases may be
523 also feasible by careful picking of arrival times in record sections [Rawlinson and Urvoy,
524 2006; Karplus, et al. 2011].

525 **4.3. Example III: A Realistic Model in Namche Barwa, SE Tibet**

526 A third test is performed on a new model that is compatible with geological reality. The
527 Namche Barwa region, located in southeastern Tibet (Figure 9), is marked by strong tectonic
528 stress, rapid rock uplift and exhumation, extremely young cooling ages, and intense
529 metamorphism and anatexis [Xu et al., 2012; Zeitler et al., 2014]. The formation mechanism
530 is still debated although several plausible geodynamic models (e.g., indenter corner, crustal
531 folding, and channel flow) have been proposed [Koons, 1995; Burg and Schmalholz, 2008;
532 Jamieson et al., 2004]. Our previous 3D teleseismic tomographic P-wave model showed a
533 complex Indian subduction style with slab fragmentation beneath the eastern Himalaya on a

534 large-scale image [Peng et al., 2016]. MT data around the Namche Barwa was inverted to
 535 produce 3D resistivity images and revealed the electrical structure of the crust [Lin et al.
 536 2017].

537 Although MT and teleseismic data has been measured over the region, no wide-angle
 538 reflection/refraction seismic surveys are available in the study area and we are currently not
 539 aware of other suitable datasets. To circumvent this issue, we use synthetic data for this test.
 540 We can obtain a resistivity model (Figure S6a) from the individual inversion of the MT field
 541 data [Lin et al. 2017]. The images exhibit several conductors in the middle crust which are
 542 mainly distributed along Indus-Yarlung suture zone (IYSZ) and to the northeast of the NB.
 543 These characteristics appear to be prominent and the anomalous region with a resistivity of
 544 approximately 1–5 $\Omega\cdot\text{m}$ has been interpreted as an accumulation of partial melt [Lin et al.
 545 2017]. To highlight the features of these anomalous bodies, the background of the MT model
 546 is modified by setting the varying background resistivities ($1.8 \Omega\cdot\text{m} < \log(\rho) < 3.2 \Omega\cdot\text{m}$) to a
 547 constant value ($\rho=310 \Omega\cdot\text{m}$). We then calculate MT synthetic data from the resulting
 548 resistivity model (Figure 9c).

549 Compared with the resistivity model, the teleseismic tomographic results [Peng et al.,
 550 2016] show a similar distribution of low-velocity anomalies in the lower crust, but they have
 551 inferior lateral resolution to the shallow structures. Therefore, the resistivity model is firstly
 552 translated into a velocity model via an empirical relationship [Moorkamp, 2017], $\log\rho = \kappa v -$
 553 1 , where κ is set to $1/2500$. A reasonable seismic model (Figure 9d) is then designed by
 554 mixing the above translated model and the pre-existing teleseismic P-wave model of Namche
 555 Barwa (Figure S6b). We use a weighted summation method to combine these two models
 556 with the same weighting factor (0.5). As a result, resistivity and velocity images show some
 557 common structure characteristics, but some details (e.g., a seismic low velocity anomaly near
 558 Motuo as shown in Figure 9d) are not matched. The velocity background is adopted from a 1-
 559 D reference model that comprises two layers over a half space with the Moho at 64 km [Zhu
 560 and Helmberger, 1996]. The real data of Moho depth (Table S1) is derived from the previous
 561 analysis of teleseismic RFs in Namche Barwa [Peng et al., 2017]. The synthetic wide-angle
 562 seismic datasets were generated from the realistic seismic model with 8 shots and 50
 563 receivers distributed in the realistic acquisition geometry (Figure 9a).

564 We apply our joint inversion approach to the synthetic datasets from the realistic model. In
 565 this joint inversion test, the MT inversion starts from a $310 \Omega\cdot\text{m}$ half-space, and all
 566 impedance tensor elements are included at 17 periods between 0.05 s and 364 s. For the
 567 seismic inversion, the initial reference Moho boundary \mathbf{H}^0 (Figure 11b) is derived from a 1-

568 degree global model of the Earth's crust (CRUST1.0) [Laske et al., 2013], and the interface **H**
569 is updated by recalculating \bar{V}_p for each iteration. The joint inversion finally reaches the
570 desired RMS ($\chi_p=1.886$ and $\chi_s=1.236$) when we select the optimal cross-gradient weights
571 ($\mu_p=1.8$ and $\mu_s=5.2$).

572 A significant difficulty when performing joint inversion with real data is the selection of
573 appropriate weights for the datasets, constraints and regularization [e.g. Moorkamp 2017].
574 By separating the selection procedure into three steps, we have found that we can produce
575 robust results with the joint inversion framework presented here. In the first step, we perform
576 constrained seismic inversions with a fixed conductivity model based on the final individual
577 MT inversion and a series of seismic cross-gradient weights (e.g., $\mu_s = 2.0, 2.4, 2.8, \dots, 7.2$).
578 This allows us to focus on the seismic inversion and the impact of the cross-gradient on the
579 velocity models. From these experiments we can choose a reasonable cross-gradient weight
580 (e.g., $\mu_s=5.4$) for the optimal seismic joint inversion model. We then repeat the procedure for
581 the MT inversion and use the final velocity model of the constrained inversion from the first
582 step as a constraint to determine the optimal cross-gradient weight for the MT part of the
583 inversion. In the final step, we fixed the MT cross-gradient weight and conduct a mutually
584 coupled MT-seismic inversion with a new series of seismic cross-gradient weights (e.g., $\mu_s =$
585 $5.0, 5.1, 5.2, \dots, 5.6$) in order to fine-tune the seismic part. The resulting weights provide a
586 good balance between structural similarity and fitting the data. Furthermore, the stepwise
587 selection procedure reduces the mutual influence of the different weights which makes
588 assessing the result difficult.

589 The solution models obtained from the separate inversions are shown in the third row of
590 Figure 10. We observe that the separate MT inversion senses the general presence of the
591 conductive anomalous bodies, but it fails to accurately delineate the boundaries of the
592 anomalies. For example, the two separate low-resistivity anomalous bodies near Bomi (i.e.,
593 L3 and L4 at 25 km depth in the true model) merge into one anomaly in the separate MT
594 inversion model as shown in Figure 10a. In contrast, the separate seismic inversion is able to
595 delineate the boundaries of some low-velocity anomalies well (e.g., the anomaly L2), but it is
596 almost insensitive to anomaly L4. This appears to be a blind area of seismic refraction where
597 ray coverage is sparse. In general, the seismic and MT results exhibit different imaging
598 sensitivity to subsurface anomalies.

599 In the joint inversion, we first perform a test with Moho perturbations and a workflow
600 without RFs. Figure 10 (the left column) shows the resulting images including at 25 km depth
601 and a cross-section. Compared to the separate inversion, the low-resistivity anomalies for the

602 joint inversion are relatively similar in shape, but they are much more intensive in space.
603 Also, the maximum resistivity of the joint inversion model is relatively higher as shown in
604 the cross-section. The recovered velocity attributes of some anomalies (e.g., the anomaly L4)
605 are relatively closer to the true value due to the contributions of the MT data. However, the
606 steep zone in the middle crust associated with the low velocity values from profile position
607 140 km to position 200 km (Figure 10c) is not clearly resolved by the joint inversion. This
608 can be probably attributed to the unsuccessful recovery of the Moho interface.

609 To produce a more consistent image of the crustal structure, we apply the coupled joint
610 inversion algorithm with the RF module to the same datasets. In the middle column of Figure
611 10, we present the resulting MT resistivity and seismic velocity images of the joint inversion
612 models. We can see a clear structural resemblance between these two models. This
613 demonstrates that the two types of parameters are effectively coupled by the algorithm. The
614 improvement in resolution of the resistivity image is clear in comparison with the separate
615 inversion. In the cross-sections in Figure 10c, the low-resistivity anomalies are difficult to
616 distinguish based on the individual inversion results. For example, conductive anomaly L2 is
617 incapable of separating from anomaly L3. In the joint inversion models, by contrast, the low-
618 resistivity anomalies are much more isolated in space and one of these anomalies (e.g., the
619 anomaly L3) is significantly concentrated.

620 The seismic shallow structure in the upper crust is also better resolved in the joint
621 inversion results. For example, the improvement of the ball-shaped low-velocity anomaly L4
622 is visible compared to the separate inversion. In addition, a minor low-velocity anomaly (i.e.,
623 anomaly L3) in the upper ~20 km emerges in the image as shown in the middle column of
624 Figure 10d. Overall, we achieve a better recovery of the geometry of the low-resistivity
625 anomalies and the distribution of the velocity values.

626 Because the interface perturbation in this test is smaller than in the previous example, we
627 cannot observe a distinct improvement of the estimate of Moho interface depth from the
628 cross-section images (Figure 10c). For the purpose of comparing the Moho interfaces, we
629 therefore investigate maps of Moho depth variation for the example. We can see that an
630 accurate Moho interface is achieved by the coupled joint inversion algorithm with the RF
631 module (Figure 11d). This Moho interface retrieved by joint inversion is very similar to the
632 true Moho interface (Figure 11a). Note that although we obtain a seemingly satisfactory
633 result of the Moho structure by only jointly inverting the MT and seismic data (Figure 11c)
634 with a prior Moho estimate, the recovery of crustal anomalies is impacted. This highlights the
635 importance of the teleseismic RF datasets in the accurate recovery of crustal structure.

636 **5 Conclusions**

637 We have developed a new algorithm for 3-D structure-coupled joint inversion of MT and
638 wide-angle seismic reflection/refraction data by assembling pre-existing MT and seismic
639 refraction travel-time tomography schemes and incorporating reflectors into the framework.
640 Our results show that an accurate estimation of the position of the Moho interface is critical
641 for this type of joint inversion. We therefore present two strategies to solve the problem of
642 accurately determining velocity parameters and Moho depth simultaneously. One strategy is
643 to independently acquire an accurate Moho interface or layered velocity model, for example
644 by 1-D joint inversion of RFs and surface wave dispersion. However, in these cases the
645 inversion results strongly depend on the quality of this prior information. Thus our preferred
646 approach is to adjust the average velocity and position of the Moho interface within the joint
647 inversion and utilize teleseismic receiver functions to update these estimates.

648 Analysis of synthetic test results reveals that the joint inversion improves the inversion
649 results in comparison with the separate inversion. Also, the combined datasets can resolve
650 crustal structure sufficiently and even, to a large degree, the trade-off between velocity and
651 Moho interface. For the realistic examples, we can conclude that the inclusion of teleseismic
652 RF data can effectively decrease the non-uniqueness for the 3-D coupled MT/seismic joint
653 inversion. The Moho interfaces need to be updated by H- κ stacking with estimates of average
654 V_p from the tomography. Then the new V_p that can be used to update the crustal velocity
655 model and the interface during the seismic inversion. This significantly contributes to a more
656 accurate estimation of Moho depth.

657 The new algorithm can be used as a tool for integrated imaging of crustal structures
658 including the distribution of resistivity and velocity parameters, the Moho interface and the
659 secondary crustal discontinuities. With suitable experiments in the future, we envisage
660 significant improvements in imaging such structures within the Earth.

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672 supporting information.

673

674 **Appendix A**

675 To minimize the objective function for MT joint inversion in Eq. (9), we evaluate the
676 partial derivatives of Ψ_{MT} and yield a series of model updates from an initial model:

$$677 \quad \mathbf{m}_p^{k+1} - \mathbf{m}_p^0 = (\lambda \mathbf{C}_m^{-1} + \mathbf{J}_k^T \mathbf{C}_d^{-1} \mathbf{J}_k)^{-1} \left\{ \mathbf{J}_k^T \mathbf{C}_d^{-1} \mathbf{X}_k - \right. \\ \left. \mu_p (\mathbf{B}_p^k)^T \mathbf{C}_\tau^{-1} [\boldsymbol{\tau}(\mathbf{m}_p^k, \tilde{\mathbf{m}}_s^k) - \boldsymbol{\tau}(\mathbf{m}_p^0, \mathbf{m}_s^0)] \right\} \quad (\text{A1})$$

678 As presented by [Siripunvaraporn et al. \[2005\]](#), and summarized in Eq. (5) and Eq. (6), the
679 normal equation in the model space is replaced by a system in the data-space:

$$680 \quad \boldsymbol{\Lambda}_k^{-1} \mathbf{J}_k^T \mathbf{C}_d^{-1} = \mathbf{C}_m \mathbf{J}_k^T \boldsymbol{\Gamma}_k^{-1} \quad (\text{A2})$$

681 Here, $\boldsymbol{\Lambda}_k = \lambda \mathbf{C}_m^{-1} + \mathbf{J}_k^T \mathbf{C}_d^{-1} \mathbf{J}_k$ is an $M \times M$ positive symmetric matrix in the model space, and
682 $\boldsymbol{\Gamma}_k = \lambda \mathbf{C}_d + \mathbf{J}_k \mathbf{C}_m \mathbf{J}_k^T$ is an $N \times N$ positive symmetric matrix in the data-space.

683 In order to apply the data-space approach to joint inversion, we need to solve the solution
684 of $\boldsymbol{\Lambda}_k^{-1}$. This $M \times M$ inverse matrix can be transformed into data-space by Woodbury matrix
685 identity and it follows that:

$$686 \quad \begin{aligned} \boldsymbol{\Lambda}_k^{-1} &= (\lambda \mathbf{C}_m^{-1} + \mathbf{J}_k^T \mathbf{C}_d^{-1} \mathbf{J}_k)^{-1} \\ &= \frac{1}{\lambda} \mathbf{C}_m - \frac{1}{\lambda} \mathbf{C}_m \mathbf{J}_k^T \left[\mathbf{C}_d + \mathbf{J}_k \left(\frac{1}{\lambda} \mathbf{C}_m \right) \mathbf{J}_k^T \right]^{-1} \mathbf{J}_k \left(\frac{1}{\lambda} \mathbf{C}_m \right) \\ &= \frac{1}{\lambda} \mathbf{C}_m - \mathbf{C}_m \mathbf{J}_k^T \left(\lambda \mathbf{C}_d + \mathbf{J}_k \mathbf{C}_m \mathbf{J}_k^T \right)^{-1} \mathbf{J}_k \left(\frac{1}{\lambda} \mathbf{C}_m \right) \\ &= \frac{1}{\lambda} \left(\mathbf{I} - \mathbf{C}_m \mathbf{J}_k^T \boldsymbol{\Gamma}_k^{-1} \mathbf{J}_k \right) \mathbf{C}_m \end{aligned} \quad (\text{A3})$$

687 where \mathbf{I} is the identity matrix, and by substituting Eq. (A2, A3) into Eq. (A1), the (k+1)-th
688 model update can be expressed as:

$$689 \quad \mathbf{m}_p^{k+1} = \mathbf{C}_m \mathbf{J}_k^T \boldsymbol{\Gamma}_k^{-1} \mathbf{X}_k - \mu_p \boldsymbol{\Lambda}_k^{-1} \left[(\mathbf{B}_p^k)^T \mathbf{C}_\tau^{-1} \mathbf{B}_p^k (\mathbf{m}_p^k - \mathbf{m}_p^0) \right] + \mathbf{m}_p^0 \quad (\text{A4})$$

690

691 **Appendix B**

692 The subspace inversion method requires the partial derivatives of objective function Ψ_{Seis}
 693 at a specified point in model space and it satisfies a basic assumption that Ψ_{Seis} is adequately
 694 smooth to validate a locally quadratic approximation about some current model:

$$695 \quad \Psi_{\text{Seis}}(\mathbf{m}_s + \delta\mathbf{m}_s) \approx \Psi_{\text{Seis}}(\mathbf{m}_s) + \boldsymbol{\gamma}\delta\mathbf{m}_s + \frac{1}{2}\delta\mathbf{m}_s^T \mathbf{H}\delta\mathbf{m}_s \quad (\text{B1})$$

696 where $\delta\mathbf{m}_s$ is a perturbation to the current model and $\boldsymbol{\gamma} = \partial\Psi_{\text{Seis}} / \partial\mathbf{m}_s$ and $\mathbf{H} = \partial^2\Psi_{\text{Seis}} / \partial\mathbf{m}_s^2$
 697 are the gradient vector and Hessian matrix respectively.

698 Disturbance $\delta\mathbf{m}_s$ is composed of a series of multi-dimensional base vectors:

$$699 \quad \delta\mathbf{m}_s = \sum_{j=1}^N \mu_j \mathbf{a}^j = \mathbf{A}\boldsymbol{\mu} \quad (\text{B2})$$

700 where, \mathbf{A} is a projection matrix and the weighting coefficient μ_j is the length of
 701 corresponding base vector \mathbf{a}^j that minimises the quadratic form of Ψ_{Seis} .

702 In order to determine the coefficient μ_j , the following Eq. (B3) in a summation form can
 703 be obtained by substituting Eq. (B2) into Eq. (B1):

$$704 \quad \Psi_{\text{Seis}}(\mathbf{m}_s + \delta\mathbf{m}_s) = \phi(\mathbf{m}_s) + \sum_{j=1}^n \mu_j \boldsymbol{\gamma}^T \mathbf{a}^j + \frac{1}{2} \sum_{j=1}^n \sum_{k=1}^n \mu_j \mu_k [\mathbf{a}^k]^T \mathbf{H}[\mathbf{a}^k] \quad (\text{B3})$$

705 The partial derivative of Eq. (B3) with respect to $\boldsymbol{\mu}$ is:

$$706 \quad \frac{\partial\phi(\mathbf{m}_s)}{\partial\mu_q} = \boldsymbol{\gamma}^T \mathbf{a}^q + \sum_{k=1}^N \mu_k [\mathbf{a}^k]^T \mathbf{H}[\mathbf{a}^k] = 0 \quad (\text{B4})$$

707 Rearranging Eq. (B4) for $\boldsymbol{\mu}$ gives:

$$708 \quad \boldsymbol{\mu} = -[\mathbf{A}^T \mathbf{H} \mathbf{A}]^{-1} \mathbf{A}^T \boldsymbol{\gamma} \quad (\text{B5})$$

709 Evaluating partial derivatives $\boldsymbol{\gamma}$ and \mathbf{H} in Eq. (10) gives:

$$710 \quad \boldsymbol{\gamma} = \mathbf{G}^T \mathbf{C}_d^{-1} [\mathbf{d}_s - \mathbf{g}(\mathbf{m}_s)] + (\varepsilon \mathbf{C}_m^{-1} + \mu_s \mathbf{B}_s^T \mathbf{C}_\tau^{-1} \mathbf{B}_s) \cdot (\mathbf{m}_s^0 - \mathbf{m}_s) \quad (\text{B6})$$

$$711 \quad \mathbf{H} = \mathbf{G}^T \mathbf{C}_d^{-1} \mathbf{G} + \varepsilon \mathbf{C}_m^{-1} + \mu_s \mathbf{B}_s^T \mathbf{C}_\tau^{-1} \mathbf{B}_s \quad (\text{B7})$$

712 and since $\delta\mathbf{m} = \mathbf{A}\boldsymbol{\mu}$ in Eq. (B2), the solution is:

$$713 \quad \delta\mathbf{m}_s = -\mathbf{A}[\mathbf{A}^T (\mathbf{G}^T \mathbf{C}_d^{-1} \mathbf{G} + \varepsilon \mathbf{C}_m^{-1} + \mu_s \mathbf{B}_s^T \mathbf{C}_\tau^{-1} \mathbf{B}_s) \mathbf{A}]^{-1} \mathbf{A}^T \boldsymbol{\gamma} \quad (\text{B8})$$

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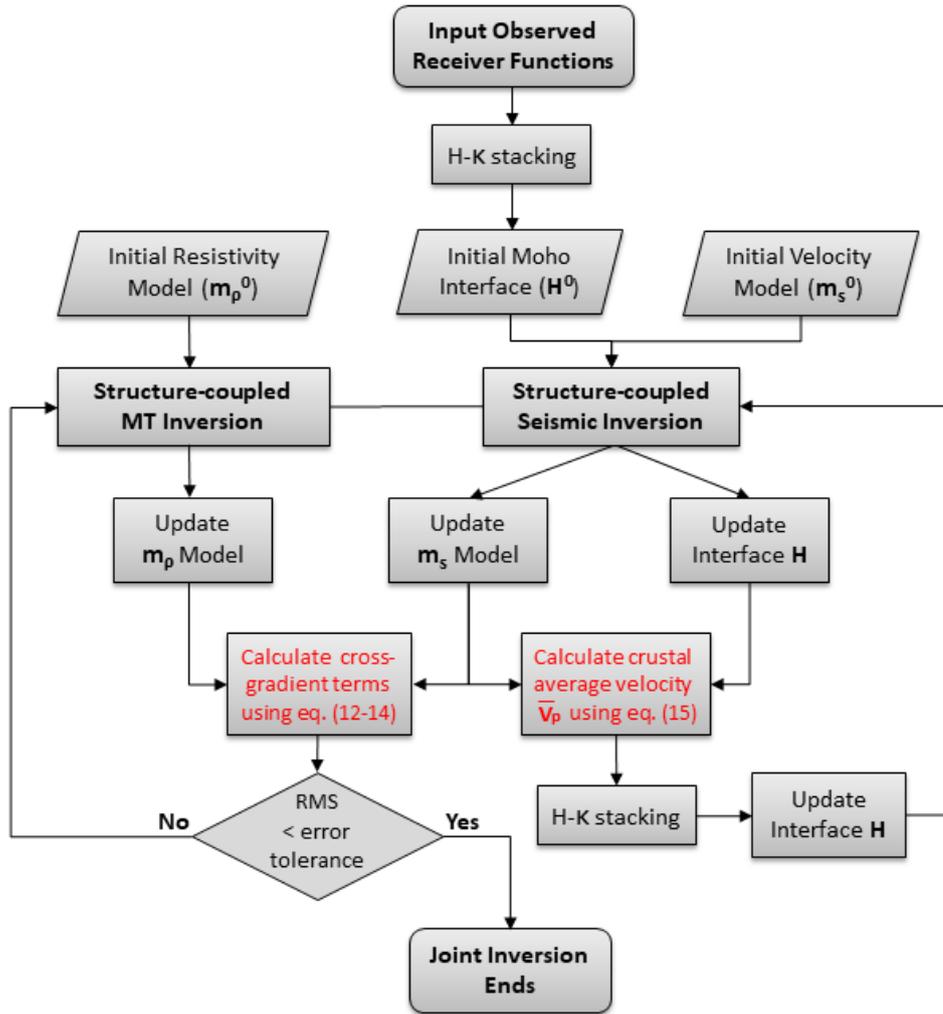
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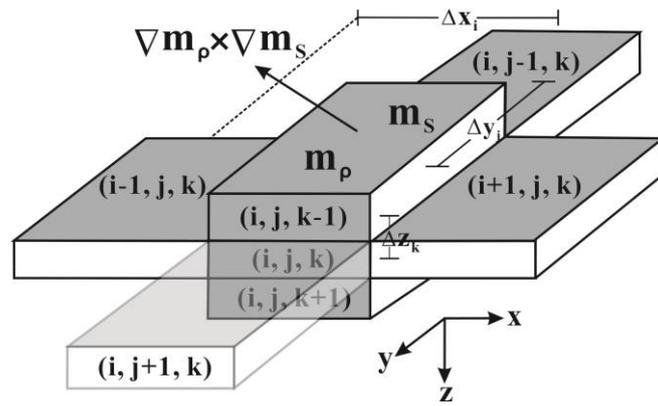
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Figure 1. Flow chart for the joint inversion algorithm including the estimation of the Moho interface through H-k stacking of RFs

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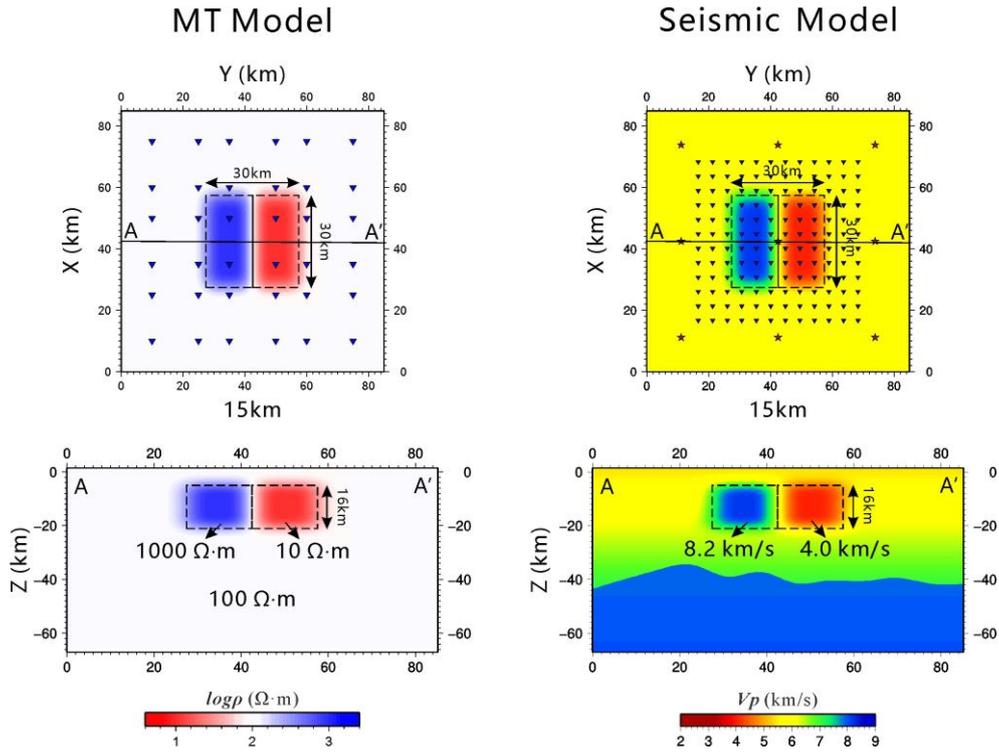


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Figure 2. Diagram of 3-D grid discretization for cross-gradient.



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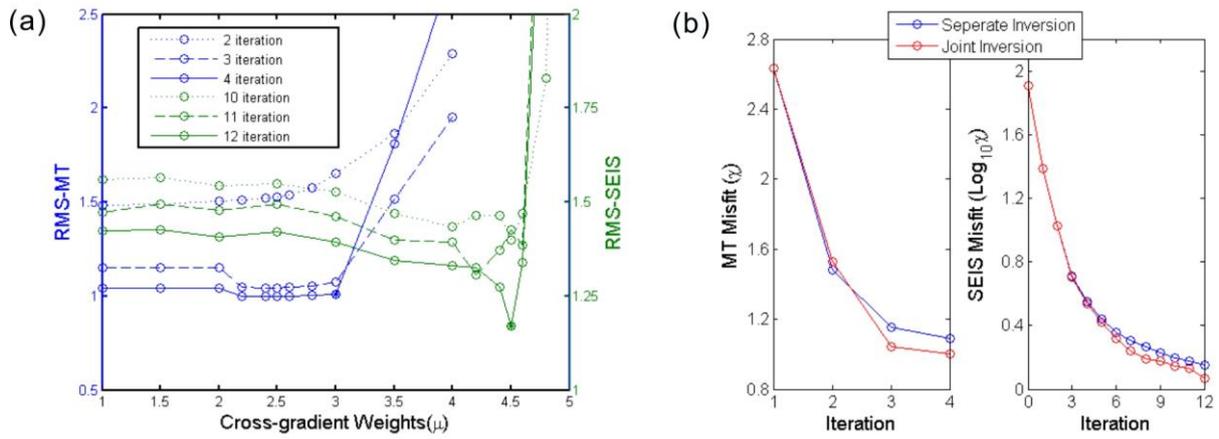
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Figure 3. Sections of true model in synthetic example I, consisting of two prisms (8 km burial depth) buried in a background. The top panel is a plan section at 15 km depth and the bottom panel is a cross-section (AA') cutting across the anomalies along E-W direction. The red stars denote sources and blue triangles denote seismic receivers or MT sites.



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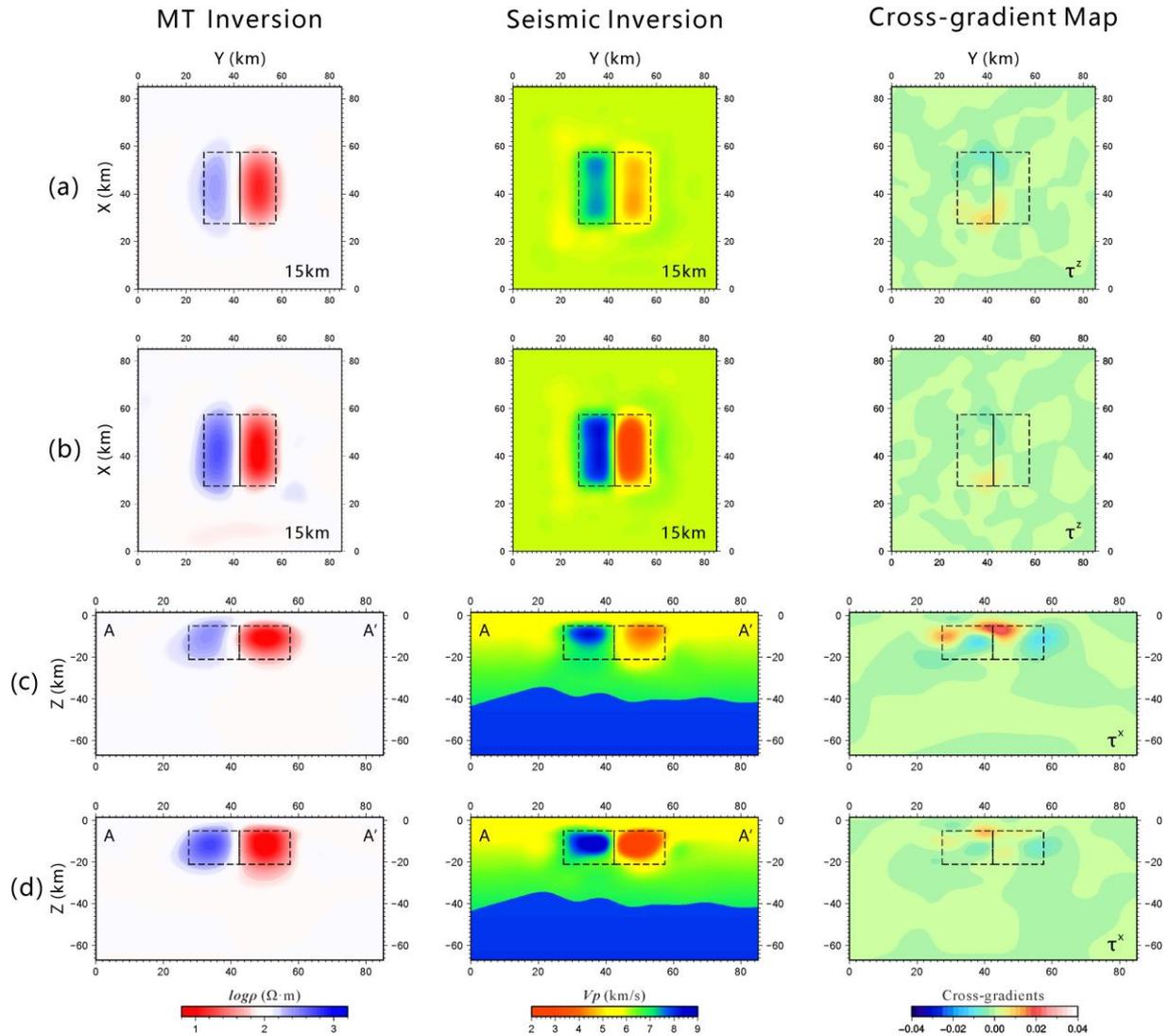
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Figure 4. Convergence curves for the last three iterations of joint inversion versus cross-gradient weights (a) and for the final inverted model versus iterations (b). Both MT and seismic joint inversion exhibit faster convergence than the separate inversion. The definition of RMS can be found in the supporting information (Text S1)



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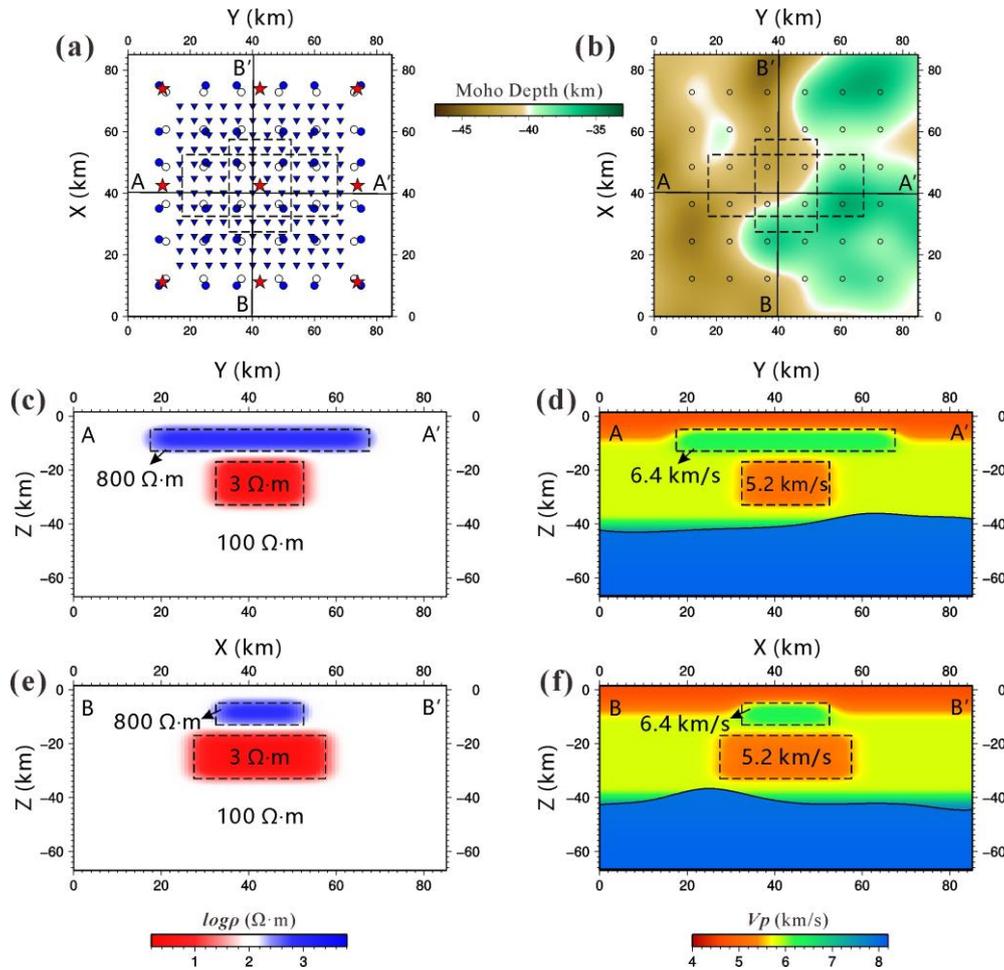
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Figure 5. Imaging results from the separate inversion and joint inversion of synthetic MT and wide-angle reflection/refraction data for a compatible model. The top panels (a)-(b) is a plan section at 15 km depth and the bottom panels (c)-(d) is the cross-section (AA') shown in Figure 3. The separate inversion results are displayed in (a) and (c) and the joint inversion results are shown in (b) and (d). Cross-gradient maps shown in the third column are plotted to examine the cross-gradients constraint and structural similarity between resistivity model and velocity model.



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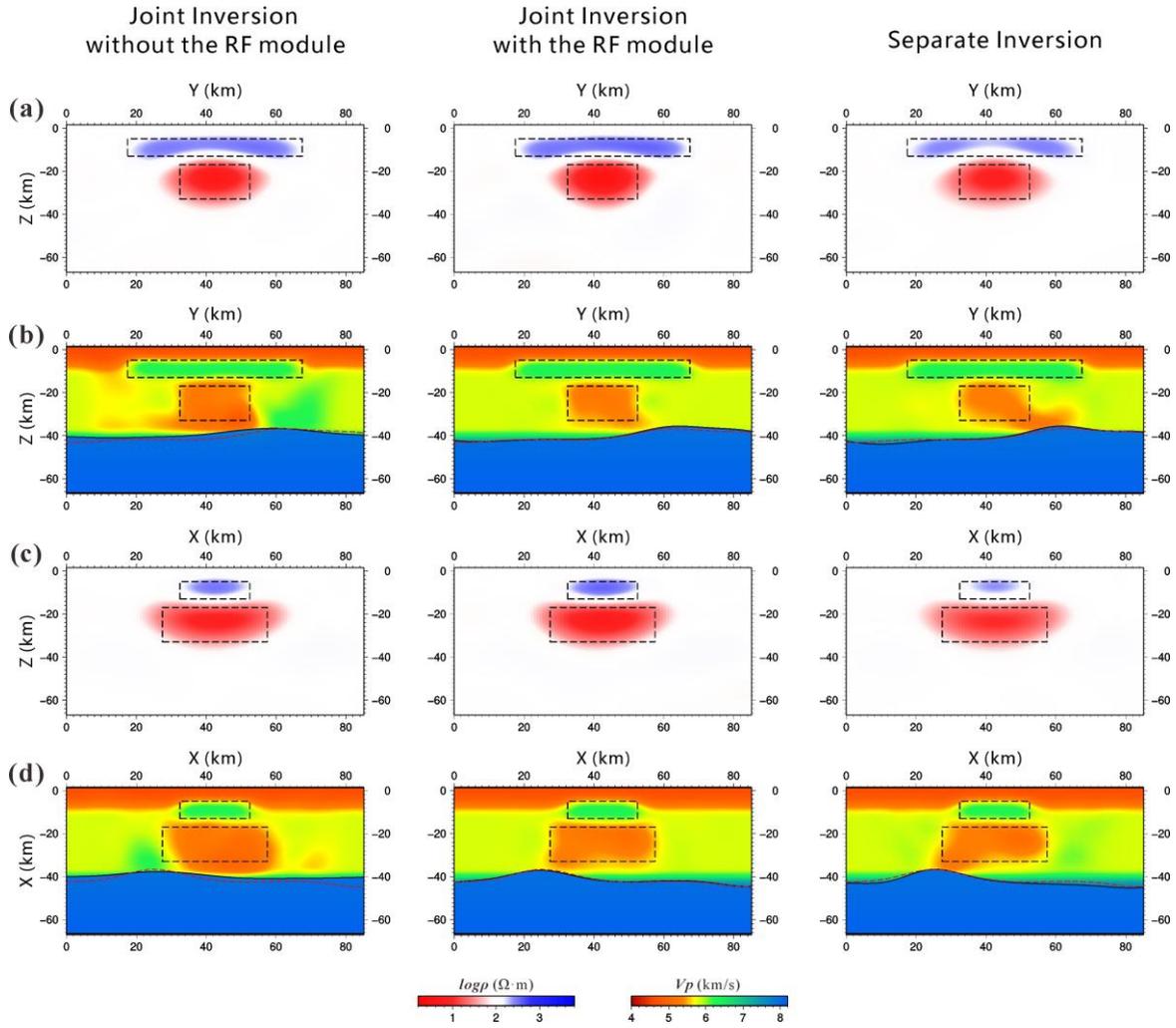
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Figure 6. Sections of true model for a realistic model test in synthetic example II, consisting of a thin layer and an underlying prism buried in a background. The top panel (a) is a plan section on the surface showing MT sites (solid blue circle), broadband seismic stations (black circle), active sources/receivers (blue triangles) and the sources (red stars) respectively; the top panel (b) shows a random Moho structure for the synthetic test; the middle panels (c)-(d) and the bottom panels (e)-(f) are cross-sections AA' and BB' along E-W direction respectively.



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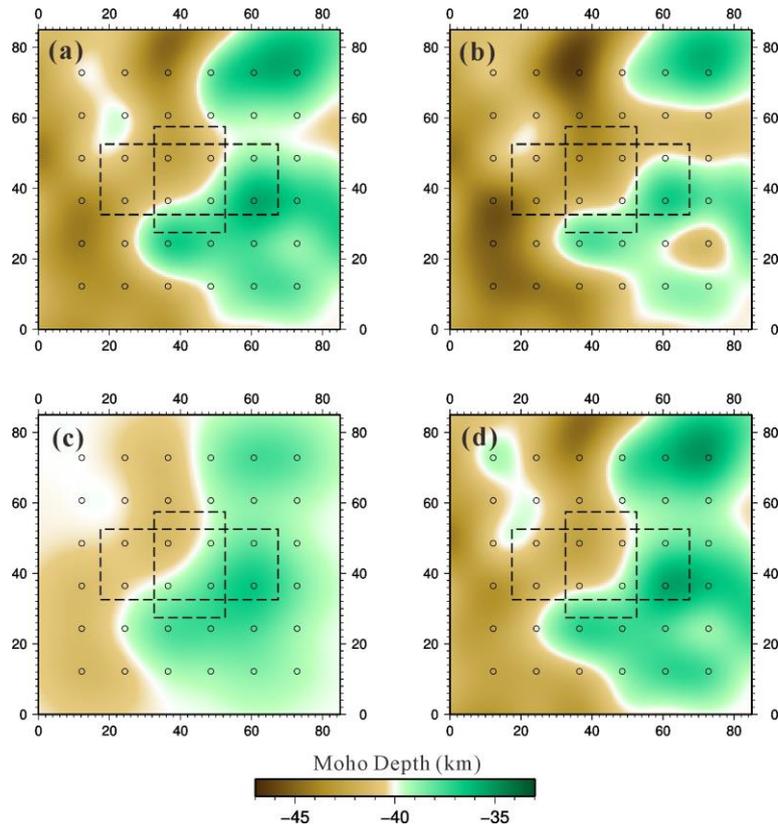
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Figure 7. Imaging results from the separate inversion and joint inversion of synthetic data generated from a complex model inverted with Moho perturbations. The panels (a) and (b) are the MT and seismic results of cross-section AA' along E-W direction, respectively; the panels (c) and (d) are the MT and seismic results of cross-section BB' along S-N direction, respectively. In the seismic images, black curve denotes inverted Moho interface and red dashed line denotes true Moho interface.

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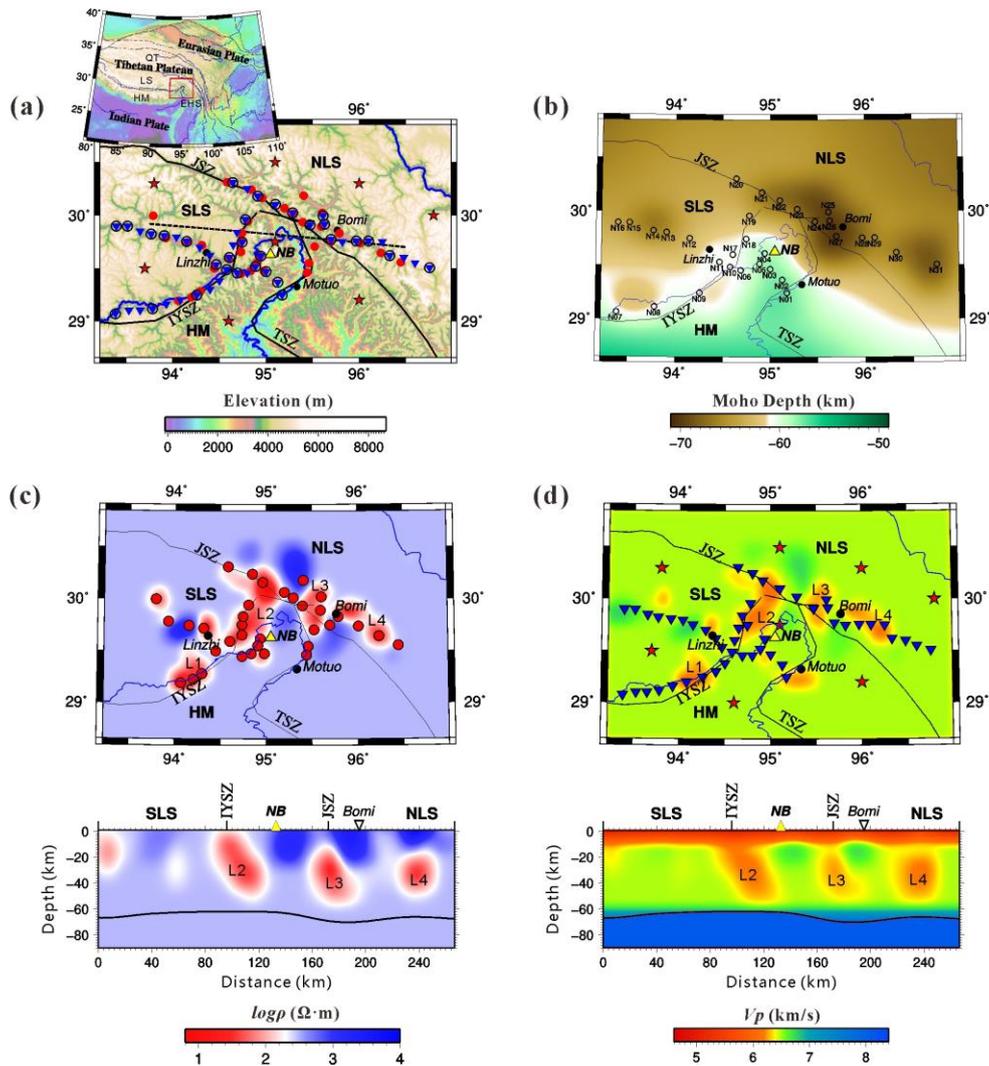
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Figure 8. Moho depth variation in synthetic example II, including (a) true Moho interface; (b) initial reference Moho depth from H- κ stacking of RFs; (c) inverted Moho interface from joint inversion without the receiver function (RF) module, and (d) inverted Moho interface from joint inversion with the RF module. The black dashed curve denotes the true shape of two anomalous prisms and Moho interface and black circle denotes broadband seismic stations.



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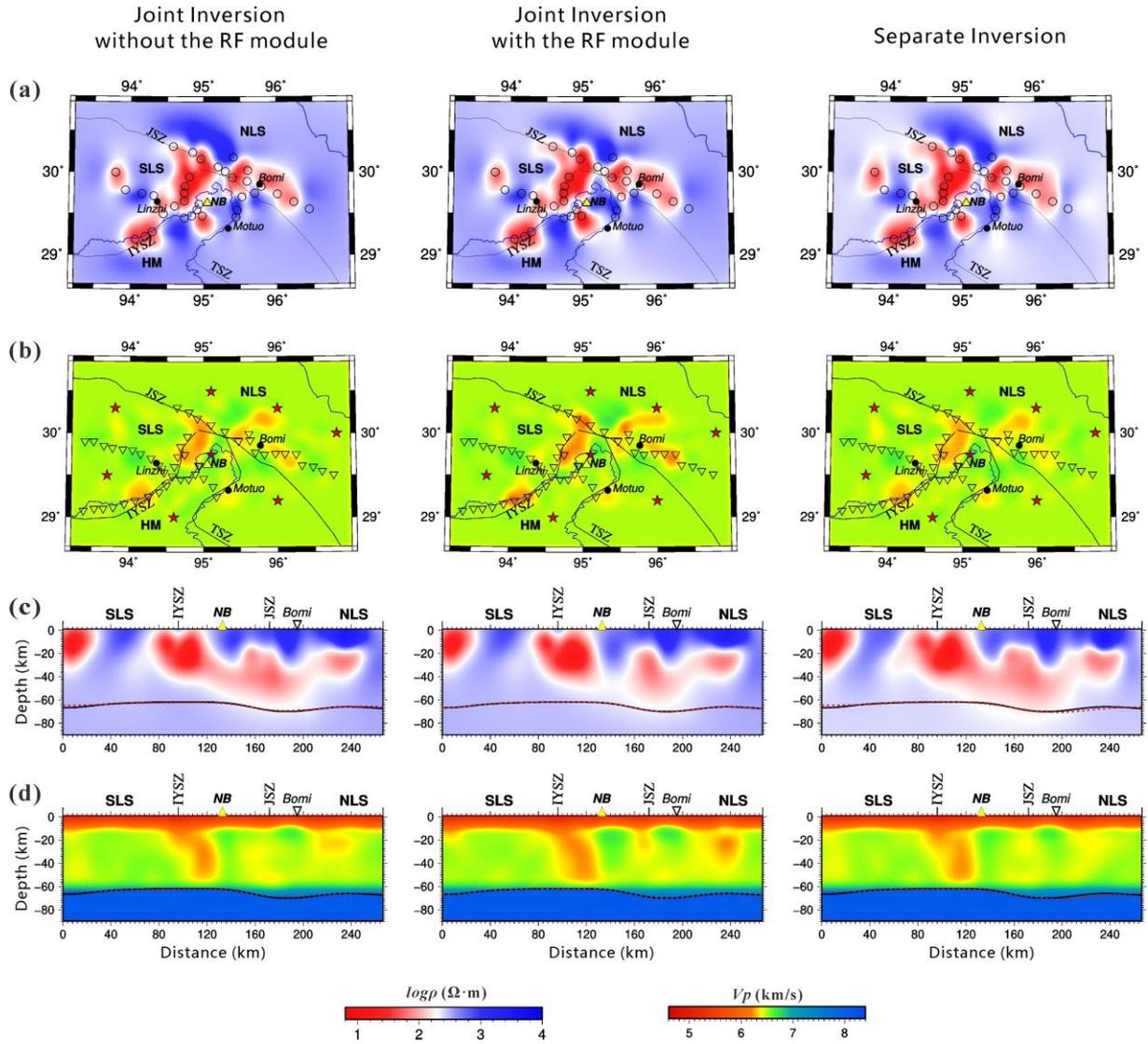
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Figure 9. (a) Locations of 35 MT sites (red circle), 31 broadband seismic stations (black circle), 50 reflection/refraction seismic receivers (blue triangle), and 8 shot points (red pentagon) on the Earth surface used in this study. The top inset map displays the location of the study area in a red box. The map shows main suture zones and large faults including: the Qiangtang terrain (QT), Lhasa terrain (LS), Eastern Himalayan syntaxis (EHS), North Lhasa terrain (NLS), Namche Barwa mountain (NB), South Lhasa terrain (SLS), Himalaya terrain (HM), Tidding suture zone (TSZ), Jiali shear zone (JSZ), and Indus-Yarlung suture zone (IYSZ). (b) True Moho depth for the realistic model interpolated by the data from CRUST1.0 [Laske et al., 2013] and H- κ stacking analysis of RFs [Peng et al., 2017]. (c) Map views of true resistivity model derived from the previous 3D MT inversion results [Lin et al. 2017]. The top panel is a plan section at 25 km depth and the bottom panel is the cross-section shown in Figure 9a. L1, L2, L3 and L4 are low-resistivity anomalies. (d) Map views of true velocity model modified from the true resistivity model and the 3D teleseismic tomographic P-wave model [Peng et al., 2016]. The position of the panels is the same as Figure 9c



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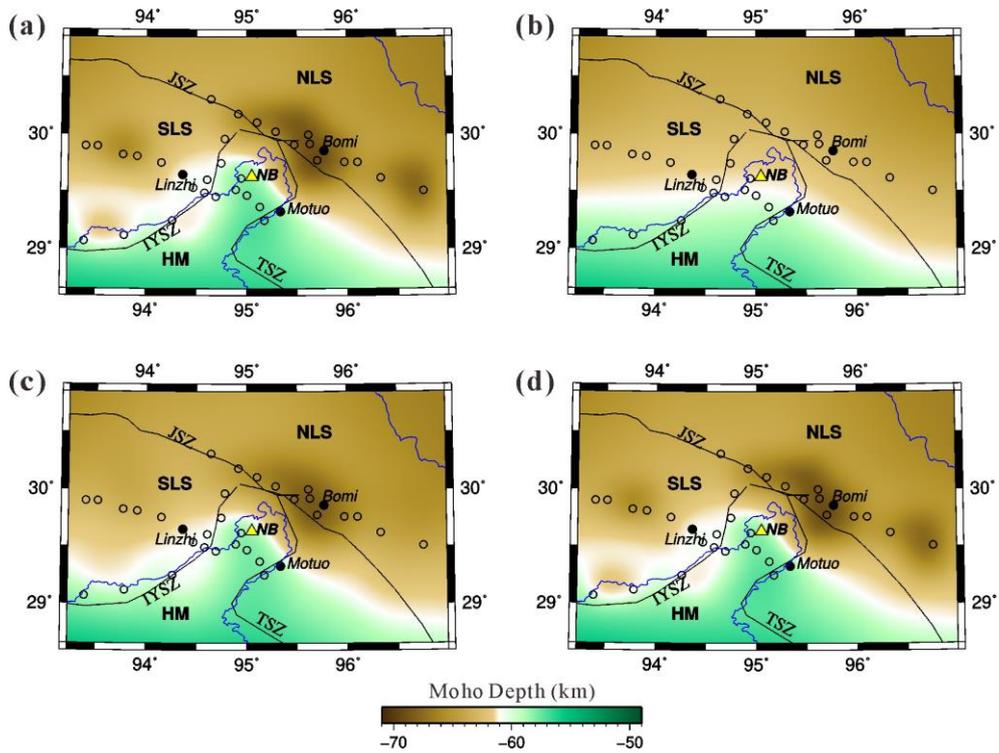
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Figure 10. Imaging results from the separate inversion and joint inversion of synthetic MT data and wide-angle seismic data in Namche Barwa. The top panels (a) and (b) are plan sections of the MT and seismic results at 25 km depth, respectively. The bottom panels (c) and (d) show the MT and seismic results as a cross-section along the line shown in Figure 9a. In the cross-section images, the black curve denotes inverted Moho interface and the red dashed line denotes the true Moho interface.



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Figure 11. Maps of Moho depth variation for the realistic example III, including (a) true Moho interface; (b) initial reference Moho depth from CRUST1.0 [Laske et al., 2013]; (c) inverted Moho interface from joint inversion without the RF module and (d) inverted Moho interface from joint inversion with the RF module. The black circle denotes broadband seismic stations.