Stochastic joint-inversion and uncertainty quantification of seismic and CSEM data

Pankaj K Mishra¹, Adrien Arnulf², Mrinal K Sen³, Zeyu Zhao⁴, and Piyoosh Jaysaval⁵

¹Geological Survey of Finland ²Amazon Web Services ³Institute for Geophysics, The University of Texas at Austin ⁴School of Earth and Space science, Peking University ⁵Pacific Northwest National Laboratory

September 17, 2024

Abstract

Uncertainty quantification in geophysical inversion is a well-recognized area of research, yet it has not become routine practice. One of the primary challenges is the computational expense of forward solvers, making robust uncertainty quantification methods like Monte Carlo or Markov Chain Monte Carlo (MCMC) impractical, particularly for higher-dimensional problems. This challenge is amplified in the case of joint inversion, where multiple types of forward solvers must be run thousands of times. We propose a stochastic joint inversion framework that integrates the Very Fast Simulated Annealing (VFSA) approach with a generalized fuzzy c-means clustering technique for effective parameter coupling. By incorporating a sparse parameterization strategy and executing multiple VFSA chains with varying initial models, we effectively mitigate VFSA's tendency to converge at the peak of the derived posterior probability density (PPD) function. The approach presented here address the inherent challenge of high computational costs for implementing joint-inversion with nonlinear sampling methods like MCMC by providing a feasible probabilistic joint inversion alternative that can integrate petrophysical information as well as geological constraints.

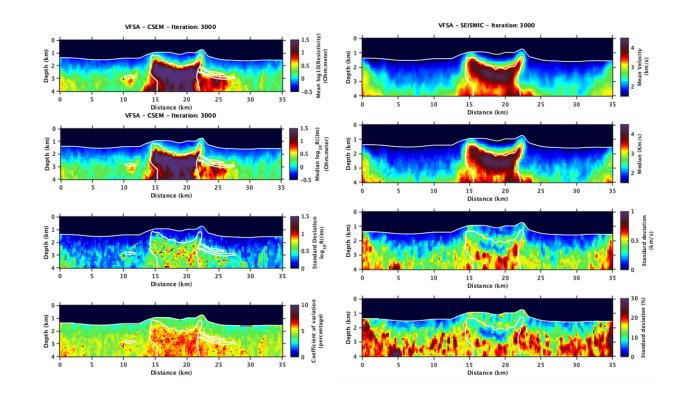


Figure 1: ThMean (a), median (b), standard deviation (c) and percentage coefficient of variance (d) for the estimated resistivity models and the mean (e), median (f), standard deviation (g) and percentage standard deviation (h) for the estimated velocity models from the joint-inversion.

Stochastic joint-inversion and uncertainty quantification of seismic and CSEM data

1

2

3

4

Pankaj K Mishra¹, Adrien Arnulf^{2*}, Mrinal K Sen ³, Zeyu Zhao^{4†}, Piyoosh Jaysaval⁵

¹Geological Survey of Finland (GTK), Finland ²Amazon Web Services, USA ³Institute for Geophysics, The University of Texas at Austin, USA ⁴School of Earth and Space science, Peking University, China ⁵Pacific Northwest National Laboratory, USA

^{*}Previously at The University of Texas at Austin

[†]Previously at The University of Texas at Austin

Corresponding author: Pankaj K Mishra, pankaj.mishra@gtk.fi

10 Abstract

Uncertainty quantification in geophysical inversion is a well-recognized area of research, 11 yet it has not become routine practice. One of the primary challenges is the computa-12 tional expense of forward solvers, making robust uncertainty quantification methods like 13 Monte Carlo or Markov Chain Monte Carlo (MCMC) impractical, particularly for higher-14 dimensional problems. This challenge is amplified in the case of joint inversion, where 15 multiple types of forward solvers must be run thousands of times. We propose a stochas-16 tic joint inversion framework that integrates the Very Fast Simulated Annealing (VFSA) 17 approach with a generalized fuzzy c-means clustering technique for effective parameter 18 coupling. By incorporating a sparse parameterization strategy and executing multiple 19 VFSA chains with varying initial models, we effectively mitigate VFSA's tendency to 20 converge at the peak of the derived posterior probability density (PPD) function. The 21 method presented here addresses the inherent challenge of high computational costs for 22 implementing joint-inversion with nonlinear sampling methods like MCMC by provid-23 ing a feasible probabilistic joint inversion alternative that can integrate petrophysical in-24 formation as well as geological constraints. 25

²⁶ Plain Language Summary

Understanding uncertainty is important in geophysics, where scientists try to figure out what lies beneath the Earth's surface by interpreting data. However, calculating this uncertainty is very challenging and is not commonly done because it requires a lot of computing power. Traditional methods like Monte Carlo or Markov Chain Monte Carlo (MCMC) are accurate but slow, especially when dealing with complex problems that use multiple types of data at once.

To solve this, we developed a more efficient method that combines a faster tech-33 nique called Very Fast Simulated Annealing (VFSA) with fuzzy clustering, a machine 34 learning method that helps connect different types of information. We also simplify the 35 process by using fewer points for the inversion through sparse sampling of model param-36 eters, and running multiple simulations with different starting points. This helps avoid 37 issue of getting stuck on one possible solution and provides a more complete picture. Our 38 approach offers a practical way to combine multiple data types and incorporate geolog-39 ical information without the high computational costs of traditional methods. 40

41 **1** Introduction

Geophysical inverse problems are known to be non-unique, which means, there ex-42 ist a number of plausible models that would fit the data. The idea behind an integrated 43 inversion is to reduce the number of possible models by using different but complemen-44 tary geophysical, geological, and petrophysical data in an unified geophysical inversion 45 framework. The term 'joint-inversion' refers to one of the many integrated (coupled) in-46 version approaches where cost functions of different methods are efficiently combined to 47 construct a joint-objective function, which is minimized while adjusting all the model 48 parameters concurrently. Since all the involved methods contribute to the model update, 49 the inversion artifacts are likely to be reduced in certain subspace of the model, which 50 is sensitive to more than one method (Moorkamp et al., 2016). There are some specific 51 challenges in the development of a efficient joint-inversion algorithm: 52

- Although a joint-inversion is likely to narrow-down number of possible solutions, the inversion problem remains non-unique and the estimated model could be suboptimal.
- In realistic models, petrophysical relationship(s) among different model param eters could be complicated, which requires an efficient coupling strategy in the joint inversion algorithm.

⁵⁹ The first challenge would be dominant if we use a deterministic method for the joint-

⁶⁰ inversion which produces a single 'best' model. A probabilistic method, however, pro-

vides many possible models which average to a final model estimation and provide un-

62 certainties in it.

Some previous works in the context of probabilistic joint-inversion have used MC 63 method (Bosch & McGaughey, 2001; Chen et al., 2004; Bosch et al., 2006; Jardani & Re-64 vil, 2009; Shen et al., 2013), Co-kriging method (Shamsipour et al., 2012), Markov-Chain 65 Monte-Carlo (MCMC) method(Rosas-Carbajal et al., 2014; Wéber, 2018), trans-dimensional 66 67 MCMC (Blatter et al., 2019), and Very Fast Simulated Annealing (VFSA) method (Kaikkonen & Sharma, 1998; YANG et al., 2002; Hertrich & Yaramanci, 2002; Santos et al., 2006). 68 Out of these, MC method is the most rigorous probabilistic approach as it samples pro-69 posal models randomly in the parameter space. The proposal models are accepted or re-70 jected based on a computed probability using the Metropolis-Hasting criterion (Metropolis 71 et al., 1953). Due to randomness in the selection of the proposal model, MC method pro-72 vides the most accurate posterior probability distribution (PPD) of the model at an ex-73 tremely expensive cost (Sen & Stoffa, 2013). 74

Unlike the MC method which is able to draw independent samples from the dis-75 tribution, MCMC method draws proposals where the next model is dependent on the 76 existing model by using the Markov-Chain. This allows the algorithms to narrow in on 77 the quantity that is being approximated from the distribution making it a less expen-78 sive alternative to the MC method. Sen and Stoffa (1996) discuss several alternatives 79 of MC method and demonstrate that a tweaked VFSA is an affordable alternative (Roy, 80 Sen, Blankenship, et al., 2005; Roy, Sen, McIntosh, et al., 2005), which can be used to 81 derive PPD without using a rigorous sampling method like MC or MCMC. VFSA is an 82 optimization algorithm based on the Metropolis-Hastings criterion. 83

There are two main differences between MCMC and VFSA as the latter uses a tem-84 perature dependent Cauchy-distribution to draw the proposal model, which tends to nar-85 row down the proposal to the previous state as the temperature decreases. Moreover, 86 the probability of accepting a 'bad' model also decreases over number of iterations and 87 becomes sufficiently low near the global minimum. The PPD derived from a single chain 88 of VFSA is inherently biased towards towards the global minimum, therefore, multiple 89 chains of VFSA are needed to get many plausible models for uncertainty quantification. 90 Although, the PPD estimated through rigorous sampling methods are more accurate, 91 the same obtained through the VFSA does provide a sweet-spot between affordability 92 and accuracy. 93

The second challenge, that is, effective coupling of model parameters has mostly 94 been discussed in the context of deterministic joint-inversion, which can be categorized as (1) structure-based coupling (Haber & Oldenburg, 1997; Gallardo & Meju, 2004) and 96 (2) petrophysical coupling (Koketsu & Nakagawa, 2002; Jegen et al., 2009). A detailed 97 review about different approaches for parameter coupling can be found in (Colombo & 98 Rovetta, 2018). In this paper, we use a guided-fuzzy c-means clustering developed by 99 (Sun & Li, 2012), which is a generalized version of the the method proposed by Lelièvre 100 et al. (2012) and has been effectively used in deterministic joint-inversion in geoscience 101 (Sun & Li, 2016a, 2016b). 102

In this paper, we introduce a probabilistic joint inversion approach for multi-physics 103 data integration, utilizing the Very Fast Simulated Annealing (VFSA) algorithm com-104 bined with a generalized Fuzzy C-Means (FCM) clustering method. Given that a large 105 number of inversion parameters would typically necessitate an impractically high num-106 ber of VFSA iterations for convergence, we employ a sparse parameterization strategy 107 to randomly distribute inversion points across the model space. We provide a detailed 108 discussion of the VFSA and FCM algorithms, explaining our rationale for their selec-109 tion in the joint inversion framework. To validate the proposed algorithm, we present 110

numerical experiments on the joint inversion of first-arrival seismic traveltime and controlledsource electromagnetic (CSEM) data for a 2D slice of the SEAM Phase I model, focusing on computing mean models and associated uncertainties. Finally, we show that, the
mean P-wave velocity model obtained from the joint inversion can be further refined using Full Waveform Inversion (FWI) (Tarantola, 1984).

¹¹⁶ 2 Forward Modeling and Cost Computation

In recent times, there has been a growing interest in the modeling and inversion of CSEM data for mapping the resistivity of the subsurface (Constable, 2010; Key, 2016; Constable et al., 2019; Lu & Farquharson, 2020). Under the low-frequency assumption (neglecting the displacement current), and quasi-static limit, the Maxwell's equations can be written as the following

$$\nabla \times \nabla \times \mathbf{E} - i\omega\mu\sigma\mathbf{E} - i\omega\mu\mathbf{J} = 0. \tag{1}$$

where **E** is the electric field, ω is the angular frequency, μ is the magnetic permeability, 122 σ , is electrical conductivity, and J is the source-term. The second-order PDE given by 123 equation (1) is the governing equation for CSEM modeling. We discretize it by using 124 the staggered-grid finite-different method (Yee, 1966; Newman & Alumbaugh, 1995). Dirich-125 let boundary conditions are applied at all boundaries of the computational domain by 126 forcing the electric field values to zero. In order to reduce the spurious data due to the 127 limited finite-domain, the computational domain was stretched by adding a thick (70km)128 highly-resistive $(10^7 Ohm.m)$ layer on top of the water layer. This additional domain was 129 discretized using stretched cells with increasing thickness along the z-direction. In prin-130 ciple, as the angular frequency reaches the static limit, the highly-resistive layer (air) causes 131 non-uniqueness in the solution, which further requires a static divergence correction. How-132 ever, for practical CSEM modeling the angular frequency is usually greater than 0.1Hz, 133 therefore, CSEM modeling does not require such corrections. A detailed description about 134 the finite-difference discritization of the equation(1) can be found in (Streich, 2009; Jaysaval 135 et al., 2014). The forward modeling kernel is parallelized by shot, frequencies wavenum-136 ber in the y-direction. 137

If \mathbf{m} is a conductivity model in a set of \mathcal{M} models, the optimization problem for CSEM can be written as

$$\mathbf{m}^{est} = \arg\min_{\mathbf{m}\in\mathcal{M}} \Phi^{CSEM}(\sigma).$$
⁽²⁾

The cost function $\Phi^{CSEM}(\sigma)$ is given by

$$\Phi^{CSEM}(\sigma) = \sum_{\mathbf{r}_s, \mathbf{r}_r, F, i, f} 0.5 W_i^F(\mathbf{r}_r | \mathbf{r}_s; \mathbf{J}, f) |\Delta F_i(\mathbf{r}_s, \mathbf{r}_r, F, i, f, \sigma)|^2$$
(3)

where F_i is the component of electric or magnetic field in the direction of x or y (i = (x, y)). ΔF is the difference between observed and computed fields at receiver location \mathbf{r}_r due the the source \mathbf{J} at location \mathbf{r}_s .

$$W_i^F = \frac{1}{|F_i^{obs}|^2 + \eta^2} \tag{4}$$

The datum weight W_i^F balances the contributions from fields at different offsets to the cost function.

For raytracing of seismic first-arrival paths, we use the shortest path method, which is an efficient and flexible approach to compute the raypaths and traveltimes of first arrivals to all points in the earth simultaneously (Moser, 1991; Arnulf et al., 2011, 2014, 2018). The forward calculation of synthetic first arrivals is fully parallelized for each re-

ceiver taking advantage of the source receiver reciprocity. The cost function for seismic

 ϕ^{SE} is given by

$$\Phi^{SE} = \sum_{i=1}^{N} \frac{\left(T_i^{pick} - T_i^{cal}\right)^2}{\sigma_i^{err}},\tag{5}$$

where T^{pick} , and T^{cal} are picked and calculated traveltimes respectively, σ_i^{err} is uncertainty in picking, and N is total number of picks.

¹⁵⁴ **3 VERY-FAST SIMULATED ANNEALING**

Simulated annealing (SA) is an optimization algorithm, which is inspired from the annealing process in Thermodynamics (i.e. (Kirkpatrick et al., 1983); see (Sen & Stoffa, 2013) for geophysical applications). The annealing is a process where a metal is heated until it melts and then cooled in a controlled way to achieve the lowest energy state. During annealing, thermal equilibrium is reached at every temperature where the set of all possible molecular configuration is given by the probability of a particular configuration of particles being in a state i

$$p_i = \frac{e^{\frac{E_i}{kT}}}{\sum_{j \in \mathcal{S}} e^{\frac{-E_j}{kT}}}.$$
(6)

Equation (6) is named the Boltzmann distribution where E_i is the energy state of the 162 configuration i, S is the set of all possible configuration, k is the Boltzmann constant 163 and T is the temperature. The SA method starts with an initial model and an initial 164 (highest) temperature. In the next step, the temperature is decreased by a predefined 165 cooling schedule, and the algorithm draws a new (proposed) model from a flat-distribution. 166 The objective function is defined as the difference between energy states of the initial 167 and the new model. If the energy state of the proposed model is less than that of the 168 previous model, the model is accepted. On the other hand, if the energy state of the pro-169 posed model is greater than that of the previous model, the model is considered as a bad 170 proposal. Since SA is a global optimization algorithm with a purpose of jumping out of 171 a local minimum, it does not discard a bad proposal model but accepts it with a prob-172 ability called the Metropolis-Hasting criterion, which is given as 173

$$P_n = e^{\left(-\frac{E(\mathbf{m}_n) - E(\mathbf{m}_{n-1})}{t_n}\right)} \tag{7}$$

where t_n is the temperature at the current step. The probability (P_n) of accepting a bad 174 proposal model is temperature dependent. As the SA algorithm proceeds to higher it-175 erations, the current temperature decreases and so does the probability. This means that 176 at initial iterations, SA would accept most of the bad proposal models but becomes par-177 simonious when the solution approaches the global minimum. The cooling schedule needs 178 to be carefully defined as it controls the trade off between the computational cost of SA 179 algorithm and its ability of finding the global minimum. A faster cooling would accel-180 erate the algorithm but a slower cooling makes sure the globally optimal solution. There-181 fore, for a complicated optimization problem the cooling schedule needs to be significantly 182 slower, which can make SA — unpractical. 183

Ingber (1989) proposed a variant of SA, called Very Fast Simulated Annealing (VFSA), which offers a significant speed-up with minimum sacrifice in the ability to find the globally optimal solution. The main difference between SA and VFSA is that instead of drawing a proposal model from a flat-distribution, the latter draws the proposal model using a temperature-dependent Cauchy-like distribution over the previously accepted model as given by

$$m_i^n = m_i^{n-1} + y_i (m_i^{ub} - m_i^{lb}), (8)$$

where m^{ub} and m^{lb} are maximum and minimum allowed values of the model parameter and

$$y_i = sgn(u_i - 0.5)t_n \left[(1 + 1/t_n)^{|2u_i - 1|} - 1 \right],$$
(9)

where u is a random number between 0 and 1. The VFSA algorithm offers some unique 192 flexibility over the SA. As such, in the initial stage of the optimization process (i.e. the 193 earlier iterations) the algorithm is set to explore a broad region of the model space. Then, 194 as the optimization process starts to converge towards the global minimum, the algo-195 rithm is set to focus on narrower regions of the model space located near the previously 196 accepted model. It is worth to be noted that in the case of multi-parameter optimiza-197 tion, VFSA allows different parameters to have their own cooling schedule and model 198 search space. 199

²⁰⁰ 4 Parameter Coupling

Clustering is a machine Learning technique that finds groups in a specific dataset, 201 where the data belonging to a group are more similar to each other than the data be-202 longing to another group. These groups in the data are called clusters. A clustering al-203 gorithm segments the data into high-density clusters such that inter-cluster members have 204 low similarity and intra-cluster data have high similarity. Clustering is an efficient tool 205 for exploring the relationship(s) between data, which, traditionally, has been a post-inversion 206 process where inversion results from single data inversions are analyzed to interpret the 207 final petrophysics and geology of the subsurface. A cross-plot between inverted param-208 eters explains the statistical relationship between model parameters and often a direct 209 relationship is derived and used as a coupling scheme in the joint-inversion. Statistical 210 coupling gets tricky when the crossplot has complex and more than one relationship be-211 tween parameters. Recently, (Sun & Li, 2016b, 2016a) proposed an efficient way of pa-212 rameter coupling by using a generalized fuzzy c-means (FCM) clustering to constrain 213 the statistical relationship of inverted parameters for several deterministic joint-inversion 214 studies. In this paper, we show that FCM can also be incorporated into our probabilis-215 tic joint-inversion framework. 216

FCM (Dunn, 1973; Bezdek, 1981) is one such clustering approach, where instead of belonging to one cluster, the data points can have a certain degree of memberships to different clusters. Clustering methods, essentially, solve local optimization problems where an optimal data segmentation is achieved by minimizing a certain cost function. The cost function for a typical FCM method is given as,

$$\Phi^{FCM} = \sum_{k=1}^{N} \sum_{i=1}^{c} (\mu_{i,k})^m (\mathbf{x}_k - \mathbf{v}_i)^T A(\mathbf{x}_k - \mathbf{v}_i), \qquad (10)$$

where $\mu_{i,k}$ are the elements of the 'partition matrix' $\mathbf{U} \in \mathbf{R}^{N \times c}$ and are termed as mem-222 bership values, which is a measure of of degree of membership of k^{th} data in the i^{th} clus-223 ter. The 'fuzzification parameter' $(1 < m < \infty)$ determines the degree of 'fuzziness' 224 in the clustered data, and the vector \mathbf{v}_i is the center of i^{th} cluster. The distance-norm 225 A determines the shape of the clusters. The standard FCM algorithm uses the Euclidean 226 norm (A = I); therefore, it detects only circular clusters in the data. However, if we 227 modify A to include variances adaptive to given data, the FCM can be generalized to 228 detect different shapes of clusters in one cross-plot. A generalized formulation of FCM 229 uses an adaptive (mahalanobis) distance-norm (Gustafson & Kessel, 1979), where each 230 cluster has its own norm-inducing A matrix given by 231

$$A_{i} = \left[\rho_{i} det(F_{i})\right]^{1/n} F_{i}^{-1}, \qquad (11)$$

where ρ_i is the determinant of the matrix A_i , and F_i is the fuzzy covariance matrix for i^{th} data as given by

$$F_{i} = \frac{\sum_{k=1}^{N} (\mu_{i,k})^{m} (\mathbf{x}_{k} - \mathbf{v}_{i})^{T} (\mathbf{x}_{k} - \mathbf{v}_{i})}{\sum_{k=1}^{N} (\mu_{i,k})^{m}}.$$
(12)

²³⁴ 5 Joint-inversion Workflow

235

247

248

249

250

We write the combined objective function for the joint-inversion as follows

$$\Phi = \Phi^{EM} + \Phi^{SE} + \Phi^{FCM} + \lambda \sum_{i=1}^{c} \| \mathbf{v}_i - \mathbf{g}_i \|_2.$$
(13)

Where Φ^{EM} , Φ^{SE} , and Φ^{FCM} are cost functions of CSEM, seismic, and FCM respec-236 tively. To adjust the contributions from each methods, we normalize the individual cost 237 functions for their target errors derived from separate VFSA inversions. This will make 238 sure that all the methods contribute equally near the global minimum and avoids free 239 parameters (weights) in the joint-inversion. The forth-term in equation (13) incorporates 240 prior information about the known geology by minimizing the distance between inverted 241 cluster centers \mathbf{v}_i , and known cluster centers \mathbf{g}_i . The parameter λ reflects our confidence 242 in the priors. The value of $\lambda = 0$ would imply that there is no prior information about 243 cluster centers and final inverted centers will be determined purely through the inver-244 sion. The iterative update scheme (Sun & Li, 2016b) for FCM centers (including the pri-245 ors) is derived as 246

$$\mathbf{v}_i = \frac{\sum_{k=1}^{N} (\mu_{i,k})^m \mathbf{x}_k + \lambda \mathbf{g}_i}{\sum_{k=1}^{N} (\mu_{i,k})^m + \lambda}.$$
(14)

In the following algorithm, we explain the probabilistic joint-inversion workflow for CSEM and seismic data for one inner loop inside the main VFSA loop. The model parameters \mathbf{m}_{res} and \mathbf{m}_{vel} represent the vertical resistivity (R) and p-wave velocity (V_p) , respectively.

251 Initialize maximum temperature t_0 , number of VFSA iterations, number of loops inside 252 VFSA iteration, random initial models: $\mathbf{m}_{res}^0, \mathbf{m}_{vel}^0$, initial random centers \mathbf{v}_i^0 253 **repeat** for n = 0, 1, 2, ..., number of VFSA iteration 254 Compute the current temperature t_n using a cooling schedule 255 Draw proposal models \mathbf{m}_{res}^{n+1} , and \mathbf{m}_{vel}^{n+1} using equation (8) Compute memberships $\mu_{i,k}^{n+1}$ using $FCM(\mathbf{m}_{res}^{n}, \mathbf{m}_{vel}^{n}, \mathbf{v}_{i}^{n})$ Update cluster centers \mathbf{v}_{i}^{n+1} using equation (14) 256 257 258 Compute $\delta E = \Phi^{n+1} - \Phi^n$ 259 If $\delta E \leq 0$ 260 261 262 else 263 $P = \exp\left(-\frac{\delta E}{t_n}\right)$ 264 Draw a random number $\{u : u \in (0, 1)\}$ 265 If P > u266 Accept $\mu_{i,k}^{n+1}$, \mathbf{v}_i^{n+1} , \mathbf{m}_{res}^{n+1} , \mathbf{m}_{vel}^{n+1} , \mathbf{m}_{vel}^{n+1} , \mathbf{m}_{vel}^{n+1} , \mathbf{m}_{res}^{n+1} , \mathbf{m}_{vel}^{n+1} 267 268 end 269 end 270 n = n+1271 end 272 273

We have normalized individual cost functions for CSEM and seismic with their respective target misfit and do not use relative weights.

²⁷⁶ 6 Test case

We apply the proposed joint-inversion workflow for CSEM and seismic travel-time data generated on a subset of SEAM Phase I model (Pangman, 2007). The subsurface

model built on the SEAM Phase I data set mimics a realistic geology of a salt-containing 279 region in the Gulf of Mexico (Fehler & Keliher, 2011). There is a massive salt body with 280 steep flanks embedded into a layered sediment environment. The velocity model has com-281 plex geometrical structures and strong velocity variations that makes seismic imaging 282 below salt: challenging. The top boundary of the salt is rugose and has a thin layer of 283 muddy salt having velocity slightly lower than the main salt body. Since we use using 284 only first-arrival travel-time data for this numerical test, we restrict our area of inter-285 est to $4 \ km$ depth. The SEAM model for this test is a subset of a 2D slice of the orig-286 inal 3D model (at north=23900 m) having the dimension of 35 $km \times 4 km$. The model 287 has a seawater layer of 0.3125 Ωm vertical resistivity and 1490 m/s p-wave velocity, and 288 the thickness of the seabed varies from $0.7269 \ km$ to $1.606 \ km$. The true synthetic mod-289 els for this experiment are shown in figure (1). The sediments on either side of the salt 290 body have some interesting formations, which are not visible in the velocity model but 291 are prominent in the vertical resistivity model. A preliminary cluster analysis of this cross-292 plot between true model parameters shows that the geology of the model can reasonably 293 be described with five clusters. We'll assume these cluster centers as a prior geological 294 information about the facies in the model. The goal of this numerical test is to perform 295 the joint-inversion of seismic and CSEM data over this SEAM model using the given petro-296 physical and geological constraints and quantify the uncertainty in the estimated mod-297 els. 298

For the seismic data, we assumed a typical ocean bottom seismometers (OBSs) pro-299 file with 34 receivers uniformly distributed every 1 km, with the seismic wavefield down-300 ward extrapolated to the seafloor (Arnulf et al., 2011, 2014). For the seismic modeling 301 we took advantage of the source receiver reciprocity. As such we are modeling 34 shots, 302 uniformly distributed at the ocean bottom between $x = 1 \ km$ to $x = 34 \ km$ and re-303 ceivers at 50 m interval. For CSEM modeling, we have used 17 sources between $x = 3 \ km$ 304 and 31 km and receivers at every 500 m. The CSEM source is an x- oriented horizon-305 tal electric dipole, which is towed 30 m above the seabed, and receivers are at seabed 306 depth. We use two frequencies 0.1 Hz and 0.25 Hz and set their corresponding max-307 imum offset to 10 km and 8 km, respectively. Forward modeling for both methods have 308 been done on regular grids $(200 \ m \times 100 \ m)$; however, for the inversion, we use a sparse 309 parameterization approach. That is, we interpolate models on 400 randomly generated 310 points for VFSA inversion. Once a model is accepted, we transform the model back to 311 orthogonal grid for forward computations. The interpolation of the model on the sparse 312 grid uses a linear radial basis interpolation. Choice of number of points for the sparse 313 parameters is a trade-off between how well it can capture the features of the model and 314 how long does it take for VFSA algorithm to converge. 315

Since the water layer is known as a prior, we perturb models only below that. For sparse parameterization, we fix 400 inversion points (same for both models) for one chain and do scattered data interpolation to transform the perturbation to regular modeling grids.

For each VFSA chain, the sparse parametrization was randomly generated (see sup-320 plementary information). As such, each starting model sampled a different spatial lo-321 cation of the model space. For this experiment, we have run 15 different chains (the ini-322 tial models and inversion points are shown in the supplementary material). For FCM 323 parameters, we assume 4 clusters (not including the water layer) in the model and pro-324 vide prior centers \mathbf{g}_i (with prior weight $\lambda = 1000$) as deduced from the true models. 325 For a real dataset, these centers would be inferred using the prior knowledge about the 326 subsurface. Figure (2) shows the resistivity and velocity model recovered in one-chain 327 of the joint-inversion. The probabilistic nature of the joint-inversion workflow allows us 328 to generate a number of models, which can be used to compute uncertainty in the model 329 via statistical analysis. We compute mean, median, and uncertainty in the joint-inversion 330 for fifteen independent chains of VFSA for 3000 iterations. Figure (3a) and (3b) show 331

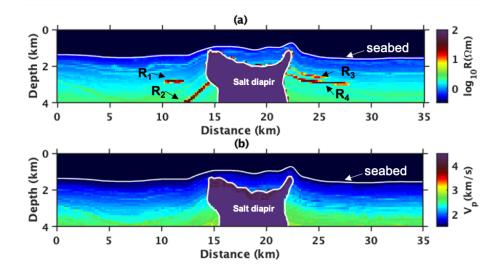


Figure 1. A 2D slice of SEAM Phase I model (a) vertical resistivity (R) on log scale and (b) p-wave velocity (V_p) . The model consist of a salt diapir in a sedimentary basin below the sea-floor (white line). There are thin reservoirs on the both side of the salt $(R_1, R_2, R_3, \text{ and } R_4)$ diapir, which are visible only in the vertical resistivity model.

the mean and median resitivity models. The top of the main salt diaper and the flanks 332 are recovered. The reservoir R_1 is also clearly visible however R_2 and the left flank of 333 the salt are not clearly resolved. Similarly, the reservoirs on the right-side of the salt R_3 334 and R_4 are recovered together and not clearly distinguished. The background sediments 335 are well-recovered. Due to the lack of EM signal in the bottom corners as well as inside 336 the salt body, we see higher uncertainties in those areas as shown in figure (3c) and (3d). 337 We notice that the reservoirs in the inverted models are slighly deeper than their loca-338 tion in the true resistivity model. As far as the velocity model is concerned, the top bound-339 ary of the salt is well resolved. The salt boundary is clearly visible as shown in the mean 340 and median models in figure (3e) and figure (3f), respectively. The background sediments 341 are well recovered except the bottom corners and lower part of the salt, which is due to 342 lack of rays passing through these areas. Given that we started with random initial mod-343 els, the estimated models from the joint-inversion show excellent agreement with the true 344 synthetic models. 345

The joint-inversion framework allows us to manually decide the weight on the prior 346 cluster centers by adjusting the value of the parameter λ . A smaller value of λ shows less 347 prior constrains and final cluster centers are mostly recovered through the inversion. A 348 higher value of λ , on the other hand, does not let the centers in the proposal model to 349 move too far away from the prior center by forcing a high prior constrains. For exam-350 ple, figure (4a) shows the cross-plot between velocity and resistivity of the true synthetic 351 model clustered by using FCM with five centers. Using these centers as priors, figure (4b) 352 and figure (4c) show the recovered petrophysics from the joint-inversion with $\lambda = 10$, 353 and $\lambda = 1000$. 354

Figure (5) shows the posterior probability density of five vertical profiles in both estimated resistivity (top row) and estimated p-wave velocity model (bottom row). Assuming the estimated values at each location (not the estimated models themselves) in all the chains have the Gaussian distribution, the PPD has been computed using histograms. In the resistivity models, the profile at $x = 12 \ km$ passes through the reservoir R_1 between 2.7-3.0 km depth. The uncertainty at the top of R_1 is less than that of the bot-

tom of R_1 , which means that the upper part of R_1 is better resolved than the lower part. 361 The vertical profile at $x = 14 \ km$ passes through a part of the reservoir R_2 between 362 $3.0-3.2 \ km$ depth. Since R_2 is close to the salt diapir, it is not as well resolved as R_1 . 363 The vertical profile at $x = 18 \ km$ passes through the salt diapir between $2.0 - 4.0 \ km$ 364 depth. This profiles shows that the uncertainties are lower near the boundary of the salt 365 and higher as the observation point goes towards the center of the salt. The uncertainty 366 between R_3 (2.4 - 2.6 km depth) and R_4 (2.7 - 2.9 km depth) in the vertical profile 367 at $x = 24 \ km$ have lower uncertainty bounds, however uncertainties inside the reser-368 voir are relatively higher. 369

Figure(6) show the convergence of individual (CSEM and seismc) as well as total (joint) cost function for 3000 iterations of 15 different chains of VFSA. The individual costs of CSEM and seismic are normalized by their target errors i.e. 1 and 0.01 respectively. The convergence plots show that the joint-inversion converges in 3000 iteration of VFSA and uses approximately equal weight of individual cost functions. This shows that VFSA is a more affordable alternative to MC or MCMC methods, which require thousands of iterations to reach convergence for posterior analysis.

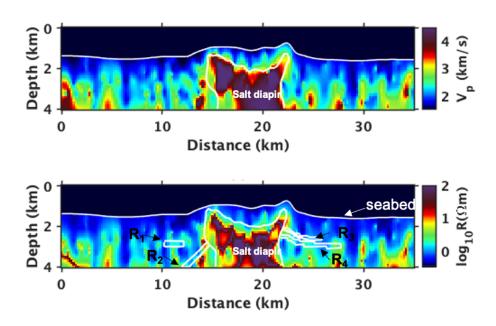


Figure 2. Inversion results for one chain: p-wave velocity (V_p) and vertical resistivity (R) models.

On of the advantage of the joint-inversion of CSEM and travel-time seismic data 377 is that the mean p-wave velocity model estimated from the joint-inversion is smooth and 378 fairly close to the true model, therefore, it can be a good starting model for FWI. We 379 modeled 16 sources placed every 1167 m over the length of the model, and receivers were 380 laid every 50 m over the length of the model. We generated synthetic data using a 4 Hz381 Ricker wavelet. We used JetPackWaveFD.jl¹ for forward modeling and Optim.jl² for FWI. 382 The initial model (mean model from the joint-inversion) is shown in figure (7a) (sam-383 pled at 10 m). We run a low frequency FWI at the same initial model sampled at 50 m. 384

¹ https://github.com/ChevronETC/JetPackWaveFD.jl

 $^{^{2}\,}https://github.com/JuliaNLSolvers/Optim.jl$

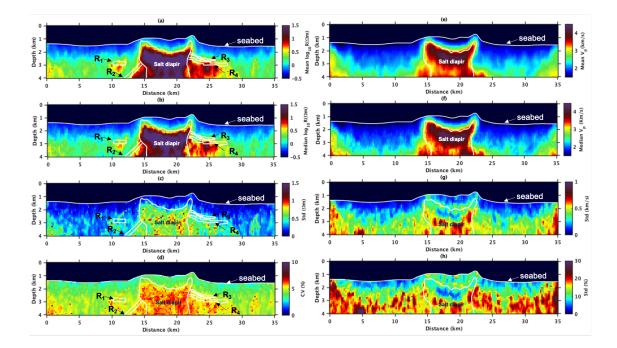


Figure 3. Mean (a), median (b), standard deviation (c) and percentage coefficient of variance (d) for the estimated resistivity models and the mean (e), median (f), standard deviation (g) and percentage standard deviation (h) for the estimated velocity models from the joint-inversion. We notice that the reservoirs in the inverted models are slighly deeper than their location in the true resistivity model.

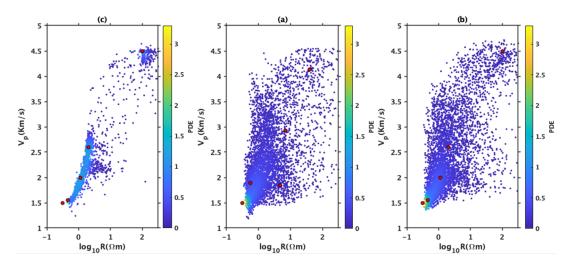


Figure 4. True (a) and recovered petrophysics with $\lambda = 10$ (b), and $\lambda = 1000$ (c). Each point is colored by the probability density estimate (PDE) for each point using kernel smoothing over its nearby points. Red dots represent the prior cluster center included in the joint-inversion as constraints. For a smaller value of λ , the centers (red dots) can move and the distance between the centers obtained from joint-inversion and prior centers are minimized over the iterations. For a larger value of λ , however, the inverted centered are forced near prior centers even in the early stages of the joint-inversion. This figure represents joint-inversion evolution for one-chain.

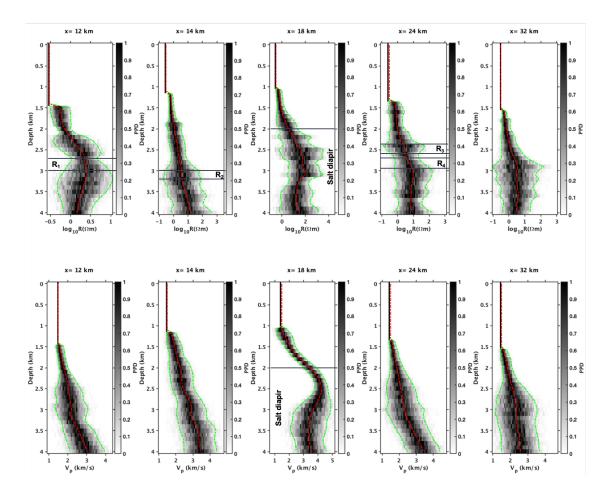


Figure 5. Posterior probability density (PPD) along vertical profiles at locations $x = (12, 14, 18, 24, 32) \ km$ for resistivity (top row) and the velocity models (bottom row). The red line shows the mean of of the models obtained in 15 different chains and green lines show the upper and lower bound of the PPD (± 2 standard deviation). The uncertainty at the top of R_1 is less than that of the bottom of R_1 , which means that the upper part of R_1 is better resolved than the lower part. Since R_2 is close to the salt diapir, it is not as well resolved as R_1 . The uncertainties are lower near the boundary of the salt and higher as the observation point goes towards the center of the salt. The uncertainty between R_3 and R_4 have lower uncertainty bounds however uncertainties inside the reservoir are relatively higher.

Figure (7b) shows the recovered model after 25 iterations of FWI and is in very good 385 agreement with the true synthetic model shown in figure (7c). The modeled data and 386 their comparison with true data have been shown in figure (7e). We flip the direction 387 of the residual and modeled data in order to help display the match with the true data. 388 Note that the data modeled in the initial model lacks a lot of reflectivity that is evident 389 in the data modeled in the true model. These missing reflectivities are recovered with 390 FWI. The FWI results from this experiemnt show that the mean p-wave velocity model 391 is a good starting model for FWI. 392

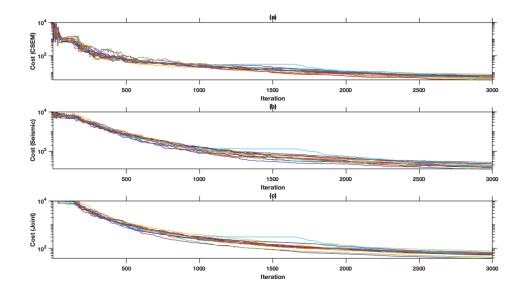


Figure 6. Convergence of (a) CSEM cost function (b) seismic cost function and (c) total cost function in the joint-inversion for 15 VFSA chains. The individual costs of CSEM and seismic are normalized by their target errors i.e. 1 and 0.01 respectively. The convergence plots show that the joint-inversion converges in 3000 iterations of VFSA and uses approximately equal weight of individual cost functions.

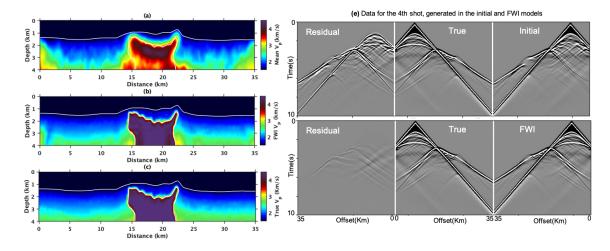


Figure 7. (a) Mean p-wave velocity model from the joint-inversion of CSEM and first-arrival traveltime data, sampled at 10 m grid. The recovered model after 25 iterations of FWI (b) and is in very good agreement with the true synthetic model (c). Comparison (e) of modeled data with true data for the initial model as well as for the FWI model shows that FWI recovered significant missing reflectivities. Note the flip in the direction of the residual and modeled data in order to help display the match with the true data. (e) shows data misfit for one shot.

³⁹³ 7 Conclusions

We have proposed a probabilistic workflow for joint inversion and uncertainty estimation, incorporating petrophysical and geological constraints. We applied this workflow to the joint inversion of CSEM and seismic synthetic data from the SEAM Phase I model. The workflow efficiently integrates petrophysical constraints and prior geological knowledge of the model. With better priors, such as facies interpreted from existing well logs, one can assign a significantly higher prior weight, causing the joint inversion to more rigorously honor the geological information.

We have demonstrated that VFSA with sparse parameterization converges faster and enables the affordable computation of multiple chains, which in turn provide uncertainty estimates in the model. The generalized FCM approach can accommodate different distance measures, which are necessary for efficient clustering based on the statistical relationships between model parameters. We believe that VFSA offers a good tradeoff between the speed of deterministic methods and the robustness of computationally expensive sampling techniques.

However, we acknowledge that the required number of iterations, although significantly fewer than those needed for MCMC methods, are still substantially higher than those typically used in deterministic approaches. For 3D inversion, a more practical application of this stochastic joint inversion approach would be to estimate starting models for deterministic inversion methods given the high computational cost of the forward solvers.

414 Open Research Section

The resistivity and velocity models used in the test case can be openly accessed from Fehler and Keliher (2011). A MATLAB function for fuzzy c-means clustering used in this paper is freely available at (Balasko et al., 2005). An open-source code of the full-waveform inversion used can be freely accessed at: https://github.com/ChevronETC/Examples. A julia implementation for VFSA joint inversion will be available at https://github.com/JuliaGeophysics/MultiphysicsInversion.jl

421 Acknowledgments

⁴²² The research was funded by TOTAL E and P, Houston, USA. The first author was par-

tially supported by Research Council of Finland

424 References

462

463

464

- Arnulf, A., Harding, A., Kent, G., Singh, S., & Crawford, W. (2014). Constraints
 on the shallow velocity structure of the lucky strike volcano, mid-atlantic ridge,
 from downward continued multichannel streamer data. Journal of Geophysical
 Research: Solid Earth, 119(2), 1119–1144.
- Arnulf, A., Harding, A., Kent, G., & Wilcock, W. (2018). Structure, seismicity,
 and accretionary processes at the hot spot-influenced axial seamount on the
 juan de fuca ridge. Journal of Geophysical Research: Solid Earth, 123(6),
 4618–4646.
- Arnulf, A., Singh, S., Harding, A., Kent, G., & Crawford, W. (2011). Strong seismic
 heterogeneity in layer 2a near hydrothermal vents at the mid-atlantic ridge.
 Geophysical Research Letters, 38(13).
- Balasko, B., Abonyi, J., & Feil, B. (2005). Fuzzy clustering and data analysis tool box. Department of Process Engineering, University of Veszprem, Veszprem.
- Bezdek, J. C. (1981). Pattern recognition with fuzzy objective function algorithms.
 USA: Kluwer Academic Publishers.
- Blatter, D., Key, K., Ray, A., Gustafson, C., & Evans, R. (2019). Bayesian joint
 inversion of controlled source electromagnetic and magnetotelluric data to image freshwater aquifer offshore new jersey. *Geophysical Journal International*,
 218(3), 1822–1837.
- Bosch, M., & McGaughey, J. (2001). Joint inversion of gravity and magnetic data under lithologic constraints. *The leading edge*, 20(8), 877–881.
- Bosch, M., Meza, R., Jiménez, R., & Hönig, A. (2006). Joint gravity and magnetic inversion in 3d using monte carlo methods. *Geophysics*, 71(4), G153–G156.
- Chen, J., Hoversten, G. M., Vasco, D., Rubin, Y., & Hou, Z. (2004). Joint inversion of seismic avo and em data for gas saturation estimation using a samplingbased stochastic model. In Seg technical program expanded abstracts 2004 (pp. 236–239). Society of Exploration Geophysicists.
- Colombo, D., & Rovetta, D. (2018). Coupling strategies in multiparameter geophysical joint inversion. *Geophysical Journal International*, 215(2), 1171–1184.
- 454 Constable, S. (2010). Ten years of marine csem for hydrocarbon exploration. *Geo-*455 *physics*, 75(5), 75A67–75A81.
- Constable, S., Orange, A., & Myer, D. (2019). Marine controlled-source electromagnetic of the scarborough gas field—part 3: Multicomponent 2d
 magnetotelluric/controlled-source electromagnetic inversions. *Geophysics*, 84 (6), B387–B401.
- ⁴⁶⁰ Dunn, J. C. (1973). A fuzzy relative of the isodata process and its use in detecting ⁴⁶¹ compact well-separated clusters.
 - Fehler, M., & Keliher, P. J. (2011). Seam phase 1: Challenges of subsalt imaging in tertiary basins, with emphasis on deepwater gulf of mexico. Society of Exploration Geophysicists.
- Gallardo, L. A., & Meju, M. A. (2004). Joint two-dimensional dc resistivity and seis mic travel time inversion with cross-gradients constraints. Journal of Geophysi *cal Research: Solid Earth*, 109(B3).
- Gustafson, D. E., & Kessel, W. C. (1979). Fuzzy clustering with a fuzzy covariance
 matrix. In 1978 ieee conference on decision and control including the 17th symposium on adaptive processes (pp. 761–766).
- Haber, E., & Oldenburg, D. (1997). Joint inversion: a structural approach. Inverse
 problems, 13(1), 63.
- Hertrich, M., & Yaramanci, U. (2002). Joint inversion of surface nuclear magnetic
 resonance and vertical electrical sounding. Journal of Applied Geophysics,
 50(1-2), 179–191.
- Ingber, L. (1989). Very fast simulated re-annealing. Mathematical and computer
 modelling, 12(8), 967–973.

Jardani, A., & Revil, A. (2009). Stochastic joint inversion of temperature and self-478 potential data. Geophysical Journal International, 179(1), 640–654. 479 Jaysaval, P., Shantsev, D., & de la Kethulle de Ryhove, S. (2014). Fast multimodel 480 finite-difference controlled-source electromagnetic simulations based on a schur 481 complement approach. Geophysics, 79(6), E315–E327. 482 Jegen, M. D., Hobbs, R. W., Tarits, P., & Chave, A. (2009).Joint inversion of 483 marine magnetotelluric and gravity data incorporating seismic constraints: 484 Preliminary results of sub-basalt imaging off the faroe shelf. Earth and Plane-485 tary Science Letters, 282(1-4), 47–55. 486 Kaikkonen, P., & Sharma, S. (1998).2-d nonlinear joint inversion of vlf and vlf-487 r data using simulated annealing. Journal of Applied Geophysics, 39(3), 155-488 176.489 Key, K. (2016). Mare2dem: a 2-d inversion code for controlled-source electromag-490 netic and magnetotelluric data. Geophysical Journal International, 207(1), 491 571 - 588.492 Kirkpatrick, S., Gelatt, C. D., & Vecchi, M. P. (1983). Optimization by simulated 493 annealing. science, 220(4598), 671–680. 494 Koketsu, K., & Nakagawa, K. (2002). Joint inversion of refraction and gravity data 495 for the three-dimensional topography of a sediment-basement interface. Geo-496 physical Journal International, 151(1), 243–254. 497 Lelièvre, P. G., Farquharson, C. G., & Hurich, C. A. Joint inversion of (2012).498 seismic traveltimes and gravity data on unstructured grids with application to 499 mineral exploration. *Geophysics*, 77(1), K1–K15. 500 Lu, X., & Farguharson, C. G. (2020).3d finite-volume time-domain modeling of 501 geophysical electromagnetic data on unstructured grids using potentials. Geo-502 *physics*, 85(6), E207–E226. 503 Metropolis, N., Rosenbluth, A. W., Rosenbluth, M. N., Teller, A. H., & Teller, E. 504 (1953).Equation of state calculations by fast computing machines. The505 journal of chemical physics, 21(6), 1087–1092. 506 Moorkamp, M., Lelièvre, P. G., Linde, N., & Khan, A. (2016). Integrated imaging of 507 the earth: Theory and applications. , 218. 508 Moser, T. (1991). Shortest path calculation of seismic rays. *Geophysics*, 56(1), 59– 509 67. 510 Newman, G. A., & Alumbaugh, D. L. (1995). Frequency-domain modelling of air-511 borne electromagnetic responses using staggered finite differences1. Geophysical 512 Prospecting, 43(8), 1021–1042. 513 Pangman, P. (2007). Seam launched in march. The Leading Edge, 26(6), 718–720. 514 Rosas-Carbajal, M., Linde, N., Kalscheuer, T., & Vrugt, J. A. (2014).Two-515 dimensional probabilistic inversion of plane-wave electromagnetic data: 516 methodology, model constraints and joint inversion with electrical resistiv-517 ity data. Geophysical Journal International, 196(3), 1508–1524. 518 Roy, L., Sen, M. K., Blankenship, D. D., Stoffa, P. L., & Richter, T. G. (2005). In-519 version and uncertainty estimation of gravity data using simulated annealing: 520 An application over lake vostok, east antarctica. Geophysics, 70(1), J1–J12. 521 Roy, L., Sen, M. K., McIntosh, K., Stoffa, P. L., & Nakamura, Y. (2005).Joint 522 inversion of first arrival seismic travel-time and gravity data. Journal of Geo-523 physics and Engineering, 2(3), 277–289. 524 Santos, F. M., Sultan, S., Represas, P., & Sorady, A. E. (2006).Joint inversion of 525 gravity and geoelectrical data for groundwater and structural investigation: 526 application to the northwestern part of sinai, egypt. Geophysical Journal 527 International, 165(3), 705–718. 528 Sen, M. K., & Stoffa, P. L. (1996). Bayesian inference, gibbs' sampler and uncer-529 tainty estimation in geophysical inversion 1. Geophysical Prospecting, 44(2), 530 313 - 350.531

- Sen, M. K., & Stoffa, P. L. (2013). Global optimization methods in geophysical inver sion. Cambridge University Press.
- Shamsipour, P., Marcotte, D., & Chouteau, M. (2012). 3d stochastic joint inversion
 of gravity and magnetic data. *Journal of Applied Geophysics*, 79, 27–37.
- Shen, W., Ritzwoller, M. H., Schulte-Pelkum, V., & Lin, F.-C. (2013). Joint inversion of surface wave dispersion and receiver functions: a bayesian monte-carlo approach. *Geophysical Journal International*, 192(2), 807–836.

539

540

541

542

543

544

545

546

547

548

549

- Streich, R. (2009). 3d finite-difference frequency-domain modeling of controlledsource electromagnetic data: Direct solution and optimization for high accuracy. *Geophysics*, 74(5), F95–F105.
- Sun, J., & Li, Y. (2012). Joint inversion of multiple geophysical data: A petrophysical approach using guided fuzzy c-means clustering. In Seg technical program expanded abstracts 2012 (pp. 1–5). Society of Exploration Geophysicists.
- Sun, J., & Li, Y. (2016a). Joint inversion of multiple geophysical and petrophysical data using generalized fuzzy clustering algorithms. *Geophysical Journal International*, 208(2), 1201–1216.
- Sun, J., & Li, Y. (2016b). Joint inversion of multiple geophysical data using guided fuzzy c-means clustering. *Geophysics*, 81(3), ID37–ID57.
- Tarantola, A. (1984). Inversion of seismic reflection data in the acoustic approximation. *Geophysics*, 49(8), 1259–1266.
- Wéber, Z. (2018). Probabilistic joint inversion of waveforms and polarity data for
 double-couple focal mechanisms of local earthquakes. *Geophysical Journal In- ternational*, 213(3), 1586–1598.
- YANG, H., WANG, J.-L., WU, J.-S., YU, P., & WANG, X.-M. (2002). Constrained
 joint inversion of magneto-telluric and seismic data using simulated annealing
 algorithm. *Chinese Journal of Geophysics*, 45(5), 764–776.
- Yee, K. (1966). Numerical solution of initial boundary value problems involving maxwell's equations in isotropic media. *IEEE Transactions on antennas and propagation*, 14(3), 302–307.