

WP5 D5.2 D13

Report on joint inversion procedures for multiple and disparate datasets (soft and hard data) with realistic subsurface structure reconstruction methods DECEMBER 2018 – Scientific deliverable Enigma ITN

WP5 - Design inverse modelling strategies for dynamic processes in complex subsurface structures

D5.2/D13: Report on joint inversion procedures for multiple and disparate datasets (soft and hard data) with realistic subsurface structure reconstruction methods

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Introduction

The use of inverse methods is common in Earth Sciences for estimating parameters from a set of field or laboratory measurements. The estimated parameters are often bulk properties of a soil or a rock (hydraulic conductivity, electrical resistivity or porosity) or a state variable such as concentration or water content. They depend on the available data and on the inverse problem.

In the field of near-surface exploration, local measurements taken in boreholes are abundant, but are not sufficient to describe the heterogeneities of the subsurface. Geophysical data can yield 2D and 3D models of the subsurface that can complement borehole information. Considering the advantages of geophysics (non-invasive with large spatial coverage but indirect information) and hydrological local measurements (more direct information but local), research for combining these two types of data has been on-going since a few decades. In the early 90s, **Rubin et al. (1992)** reported a comparative studies between a 1D geophysical-hydrologic inverse model and a hydrologic-only inverse model using seismic properties to identify hydraulic properties. Their results showed an improvement with the coupled approach compared to the hydrologic inverse problem results. Since then, the two disciplines became what is known today as the field of *Hydrogeophysics (see also Binley et al., 2015 for a review)*.

Although results obtained in hydrogeophysics since the 90s are promising, there are still limitations and a lack of application of joint inversion for real field cases (**Huisman et al. (2009)**, **Binley et al. (2015)**). One of the limitations of joint inversion comes from the solution of the inversion problem itself. Inverse problems are ill-posed and their solution are non-unique. Often, a "regularization" is applied since the 60s to stabilize the inverse model during optimization, but this regularization smoothes the inverse model and therefore does not honor the subsurface heterogeneities.

When dealing with subsurface systems we usually face the problem of capturing spatial heterogeneity at relevant scales to study a certain dynamic process of interest. Therefore, we aim to find a way to input all the information that contributes to the understanding of this process in the subsurface, which may include geological information (depositional environment, presence of fractures, degree of weathering, etc.) and also field measurements or data (core sampling, geophysical data, hydrological data, etc.). Coupled joint inversion is a procedure which uses all datasets simultaneously to solve the inverse problem. This approach has showed its benefits over the uncoupled approach in which datasets are treated independently, and is the approach that will be explored in Workpackage (WP) 5. Plus, joint inversion allows the introduction of "a priori" geological knowledge in the model construction using various methodologies to simulate geologically-based models (process-, object-, training image- and variogram-based).

The challenges addressed in WP 5 are (1) to enhance our capability to represent complex sedimentary and fractured structures that determine the spatial distribution of preferential flowpaths, the dispersion of dissolved chemical species and the related fluxes and reaction rates, and (2) to infer the flow transport and reaction processes in a consistent fully coupled framework rather than relying on decoupled geophysical inversion and hydrological interpretation of the tomograms.

Early Stage Researchers (ESRs) are working towards developing (i) new strategies for representing complex architectures of sedimentary and fractured media, based on training images, multi-point geostatistics, and genetic approaches; (ii) inversion frameworks that integrate data of diverse nature, and model uncertainty; (iii) novel tomographic inversion approaches for 2D and 3D imaging based on fully coupled inversion of time lapse ERT of tracer motion, hydraulic tomography and heat tracer tests.



This deliverable is organized as follows: first, we will address the development of joint inversion for the near-surface highlighting challenges and limitations, then we will review realistic subsurface reconstruction methods using joint inversion, and finally we will address how ENIGMA will contribute in this field of research.

1. Joint Inversion in near-surface environments

1.1 More than 25 years of development

Inverse problems for near-surface environments are often ill-posed in the sense of Hadamard, meaning that the solution is neither unique nor stable nor even exist (**Arsenin**, **1979**). Early in the 70s, several disciplines in the Earth sciences concentrated efforts in developing methodologies that made possible the solution of inverse problem. In Geophysics, **Zhdanov (1993)**, in his tutorial for the regularization in inverse theory, states that geophysicists stabilized the problem by using a set of geologically reasonable set of parameters as a starting model; or by applying regularization algorithms (**Tikhonov (1977, 1987)**) with implementation of 'a priori' knowledge (**Zhdanov (1988)**). In the field of hydrology, **Korganoff (1970)** and **Emsellem and de Marsily (1971)** recognized that the inverse problem could be stabilized by introducing a regularization term. Later, **Gavalas (1976)** proposed a Bayesian approach to view model parameters as random variables with a known constant mean and a prescribed covariance matrix. This set the ground for the development of other types of regularization which included a priori knowledge in the inverse problem using geostatistics (**Neuman (1976, 1979, 1982)**, **Kitanidis and Vomvoris (1983)**, **Hoeksema and Kitanidis (1984)**, **Carrera and Neuman (1986)**).

Parallel development of inverse problems in the two disciplines is known since the 70s to merge today in what is known as joint hydrogeophysics inversion. We should note that the term "joint inversion" in geophysics literature is used both for structural joint inversion (inversion of several types of geophysical measurements) and petrophysical joint inversion, in which geophysical and process-based data are related through petrophysical relationships, and we will focus on the latter on this report.

1.2 A brief review of the theory behind the inverse problem

Solving an inverse problem requires first to obtain the solution of the forward problem to obtain the numerical data that needs to be compared to the observed data. With numerical methods, Earth is discretized in a finite set of parameters fine grid and a parameter is estimated for each cell of the grid or for certain regions of the grid (the process of decreasing the number of parameters to be estimated is called "parametrization"). A continuous distribution of parameters may be possible using analytical models for certain types of situation.

The inverse problem is usually formulated as an optimization problem where one minimizes the difference between numerical and experimental results (deterministic approach) or maximizes the likelihood function of a set of parameters (probabilistic approach) **(Hadidi and Gucunski, 2009)**. There are many numerical methods to solve such problems : linear or non-linear least-squares, maximum plausibility, Monte-Carlo method, simulated annealing, or genetic algorithms.

The deterministic approach yields a single best fit model between modeled and observed data. Here, the uncertainty of the model is computed based on an error propagation approach. The probabilistic



approach doesn't yield a single solution, but the 'a posteriori' probability density function (in terms of Bayesian theory) describing the best fit model, and thus, a measure of its uncertainty.

1.3 Combining different types of data

Data are often classified as soft (geophysics, core analysis...) and hard (borehole) data depending on their direct or indirect nature. In the inverse problem, the objective function compares experimental and numerical measurements. Depending on the nature of the experiment, the data can include heads, concentrations, resistivities, seismic/electro-magnetic waves travel-times, or other. To weight the data according to their types (soft or hard), Medina and Carrera (2003) used for example the expected value of the likelihood function to derive the relative weights of different types of information. Before the practice of joint inversion, geophysics was mainly used to build the structural conceptual model but, thanks to time-lapse surveys, geophysics is seen as a tool to constrain hydrological models. In the static mode, geophysics was used to define stratigraphic units which share the same hydrological properties, and to define zones in which the hydrological properties could be considered constant. Nowadays, geophysical measurements are recognized as a source of information that can constraint near-surface processes. Hydrogeophysical inversion has been used for salt tracer tests in saturated aquifers (Pollock and Cirpka, 2012) because ERT response is sensitive to changes in fluid conductivity, and therefore, to salinity. In time-lapse inversion, changes in geophysical data are correlated with hydrological processes, but as there are severe resolution problems in the geophysical methods (Day-Lewis et al., 2005) (especially, ERT which is based on low frequency processes) these time-lapse inversions can result in loss of mass-balance (e.g. inferred plumes being unphysical in tracer tests, (Day-Lewis et al., 2007)). Time-lapse has the same challenges than the static geophysical images, such as resolution limits, smoothing constraints and mass balance issues. Nevertheless, the objectives of time-lapse geophysical surveys are increasingly quantitative (Singha et al., 2014), and it is state-of-art to use time-lapse results for quantitative interpretation.

There are two main approaches for inverting hydrogeophysical data: the *uncoupled* and the *coupled* approach. **Hinnel et al. (2000)** described the uncoupled approach as a three steps procedure: first, the inversion of geophysical data alone; second, the use of a petrophysical relation to relate the geophysical property to the hydrological state variable; and third, calibrate the hydrological model using direct and inferred hydrological measurements. This may also be referred to as sequential inversion or cooperative inversion (Moorkamp et al. 2006), meaning the inversions of single datasets share information between each other to estimate the hydrological parameters. One of the advantages of using this approach is the single dataset objective function. There is no need to have relative weights between data because they are independently inverted. There are important drawbacks, such as: the propagation of errors throughout each step of the inversion procedure (wrong appraisal of geophysical data errors, erroneous petrophysical relations); the large parameterization of geophysical inverse problems; and, the use of the regularization operator to solve the inverse problem, not suitable for the estimation of hydrological properties. For example, regularization may not respect the mass balance.

The coupled joint inversion makes use of all data simultaneously in an optimization process if a deterministic solution is sought. The geophysical parameters and hydrological state variables are coupled through a petrophysical relation and data are simulated in the forward hydrogeophysical operation of the inversion. The challenge of finding the good petrophysical parameters remains



present, but bias linked to regularization is avoided. For example, the issue of the mass balance is overcome. The mass conservation principle is taken into account in the simulation of geophysical images through the hydrological modeling. **Singha et al. (2014)** stressed in their review on the subject that important mass-balance problems can come from erroneous or over-simplistic assumptions on the petrophysical relations, an issue that will only be confirmed in the following years **(Binley et al., 2001; Singha and Gorelick, 2005, Müller et al., 2010).**

Huisman et al. (2009) highlights a lack of application of joint inversion in real field datasets, being at the time the most cited study cases the ones from Kowalsky et al. (2005), Deiana et al. (2008) and Looms et al. (2008). Kowalsky et al., (2004) linked an unsaturated flow simulator and a GPR forward solver to relate permeability to water content. Scholer et al. (2011; 2012) used a Markov chain Monte Carlo (MCMC) inversion to study the influence of prior information on estimated hydraulic properties. The results showed that geophysical data contained valuable information, but that better results were obtained with prior distributions that were informative on parameter correlations. Looms et al. (2008) used 1D flow simulations with ERT and GPR data to invert for permeability. The forward simulators were linked to the hydraulic simulator using homogeneous and theoretical petrophysical relationships. Irving and Singha (2010) found that ERT mainly improved the estimates of the spatial correlation length. Jardani et al. (2012) included ERT, self-potential and tracer concentrations in the inversion and found that all three datasets contained valuable information on permeability.

1.4 Current challenges and limitations

Field studies show joint inversion is certainly a site specific procedure, due to heterogeneities in the soils that cause important changes in the physical processes. It is clear now that using generic petrophysical parameters to couple hydrological and geophysical parameters is not the good approach; and, that the smoothed images resulting from geophysical data inversion is not suitable to capture hydrological model variations.

Binley et al. (2015) dedicated a section of their review to the limitations of the methods. They agree on the resolution problem, adding that smoothed images do not honor the geostatistical information that an interpreter has about the subsurface. They also point out computational constraints, because inverting for thousands of parameters or running hundreds of model realizations is computationally expensive. They discuss the impact of poorly known petrophysical relations in the study sites. **Linde and Doetsch (2016)**, also tackled in their review this issue and claim that the uncertainties related to the assumptions on the petrophysical parameters, the errors related to them and the use of the parameters for data at different scales is a problem that is seldom addressed.

The need of a prior assumption about the hydrological model when doing joint inversion is a limitation to the joint inversion procedure. **Ferré et al. (2004)** in his early attempts to use joint inversion concluded that the success of the inversion depended on the reliability of the hydrological model, and that, this dependence on the goodness of the hydrological knowledge, made the inversion lose its relevance.

Many questions arise in regards to this subject:

• Petrophysical relations, do we know how to establish them at the scale of the field sites? And the parameters, should they still be considered constant among geological units?



- For what parameters should we invert for and when? To what purpose ?
- How do we address uncertainty quantification ?
- Joint inversion is a computationally expensive procedure. Which one of all these limitations could we sacrifice to make the procedure useful for real applications?
- A good hydrological model is one that reflects the heterogeneities of processes in the subsurface. Smoothed images from geophysics or over-simplistic interpolated images from the point-measurements are, nevertheless, the ones available. Which methods could we use to create realistic subsurface models?

2. Structure Reconstruction: towards realistic subsurface models

2.1 Integrating information related to structure

When dealing with subsurface systems we usually face the problem of capturing spatial heterogeneity at relevant scales to study a certain dynamic process of interest. Therefore, we aim to find a way to input all the information that contributes to the understanding of this process in the subsurface, which may include geological information (depositional environment, presence of fractures, degree of weathering, etc.) and also field measurements or data (core sampling, geophysical data, hydrological data, etc.). The former is related to structure and different methods have been proposed to integrate it with data in both deterministic and probabilistic inversion. Two main strategies have been used to deal with structure in inversion: (1) consider structural constraints in the model, and (2) sample prior models by means of algorithms that build the expected structures.

As previously mentioned, the first strategy was proposed for deterministic inversion of geophysical data by **Constable et. al (1987)** and has been widely applied since then, because the constraints are used as regularization terms to solve ill-posed inverse problems **(Tikhonov and Arsenin, 1977)** and one is able to obtain a unique model. However, by doing so, minimum-structure models are favored which, depending on the selected regularization term, have transitions that are, e.g., smooth **(deGroot-Hedlin and Constable, 1990)** or sharp **(Farquharson and Oldenburg, 1998, Portniaguine and Zhdanov, 1999)**. One can also impose constraints in the parameter covariance matrix **(Maurer et al., 1998)** which may include imposing a variogram model during inversion **(Johnson et al., 2007)**. **Caterina et al. (2014)**, present a comparison of different strategies to incorporate prior information in ERT and they found geostatistical constraints is particularly useful when it is possible to compute correlation lengths from independent data (e.g. borehole geophysical logs). In probabilistic inversion, these structural constraints have been applied by **Rosas-Carbajal et al. (2014)** and **De Pasquale and Linde (2017)** to limit the possible realizations in the prior distribution.

The second strategy can easily be integrated in probabilistic inversion by considering the prior model distribution. **Linde et al. (2015)** provide a review on different methods to simulate realistic structures for these prior models in hydrogeological and geophysical inversion. They classify existing methodologies to simulate geologically-based models in four: process-, object-, training image- and variogram-based. **Mosegaard and Tarantola (1995)** present a Markov-chain Monte Carlo methodology that is able to integrate prior models generated by any of the mentioned strategies.



2.2 Joint inversion and structure reconstruction

Once we choose how to quantitatively input our geological (structural) conceptual knowledge of the subsurface system of interest, we may use inversion to integrate information that is given by field data. When data from different sources is available, we will consider joint inversion to use the complete dataset. As mentioned in Section 1.b, we could either use an uncoupled or a coupled approach. In joint deterministic inversion, the coupled strategy to consider structure is by using constraints along with a joint objective function, which may have different weights for each type of data. Linde et al. (2006) used constraints in the parameter covariance matrix to perform inversion with cross-borehole ERT and GPR. Though strictly not adding any more structural information than the one contained in the data, the cross-gradient structural inversion proposed by Gallardo and Meju (2004) adds the conceptual assumption that when using a joint dataset one could consider that all data comes from the same distribution of subsurface materials, then corresponding spatial changes in geophysical properties should be similar.

If our objective is to integrate time-lapse data of a transient process (e.g. breakthrough of contaminant plume): (1) the uncoupled approach is usually based on difference inversion (LaBrecque and Yang, 2001) and (2) the coupled approach will consider explicitly the simulation of the process and its geophysical response (Hinnell et al., 2011). Some studies have dealt with structure and time-lapse data by means of different regularization schemes: cross-gradient constraints (Doetsch et al., 2010), minimum support (Fiandaca et al., 2015), and minimum gradient support (Nguyen et al., 2016).

A coupled joint probabilistic inversion will use the joint dataset by a combined likelihood function **(Irving and Singha, 2010)**. We can include structural uncertainty in this coupled approach which will result in a better quantification of uncertainty but may prohibitively increase the computational demand. In order to integrate structural prior information, a Bayesian approach on all variables involved was proposed by **Park et al., (2013)**. They reduce computational demand by proposing a decomposition of the complete inversion in two steps where the first deals only with structural uncertainty. This methodology was successfully applied to a joint dataset of hydrological and geophysical measurements by **Hermans et al. (2015)**.

3. ENIGMA projects outlook

3.1 Greeting today's challenges

The scientific challenges of the deliverables in the ENIGMA projects are related to issues limiting the growth of joint inversion methods for real life applications: uncertainty of the conceptual model and of the petrophysics are two main bottlenecks. In Work Package 5, as in other Work Packages, ESRs are investigating several approaches, probabilistic and deterministic, for efficient data integration in space and time. It is important to emphasize that joint inversion procedures are not the only way to estimate subsurface parameters, and that a lot of discussion is going on now in the scientific community about the actual relevance of the estimation of certain parameters distribution when we could predict system states or project objectives (either by data assimilation or machine learning techniques). It is only natural that the ENIGMA ITN puts efforts in taking a step forward in joint inversion techniques, but also explores such other possibilities:

• Prediction of hydrological states through data integration using a probabilistic approach called Ensemble Kalman Filters is being investigated by ESR13.



- Joint inversion of hydrological and geophysical data is investigated by ESR 14, with a focus on the insertion of geological constraints in the deterministic inversion approach.
- Model uncertainty quantification is investigated by ESR15, using Bayesian Evidential Learning (BEL) to predict future system states from existing datasets.

In other Work Packages, although not directly working in joint inversion procedures, other ESRs are conducting research on topics related to the combination of geophysical and hydrological datasets (ESR4), and to the upscaling of petrophysical parameters (ESR9).

3.2 Expected Results

If the objectives of the deliverable are fulfilled by 2020, the scientific community would benefit from (and not exclusively):

- Methodologies for obtaining subsurface images, which are realistic enough to explain geological heterogeneities and design conceptual models.
- Methodologies for integrating soft and hard data by conducting joint inversion or other parameter estimation techniques, such as BEL or Ensemble Kalman Filters.
- Best practices for conducting experiences that will need data integration.
- Procedures to estimate model uncertainty in both probabilistic and deterministic approaches.
- Transparent computer algorithms for the use of the scientific community.
- Publications about data integration methods with real field applications.

3.3 Main innovations of the developed joint procedures

ESR 13 plans to develop a fully coupled 3D inversion procedure for the joint analysis of field-scale tomographic data sets from multiple investigation techniques (geoelectric and flow models). In this context, Ensemble-Kalman methods will be adapted as inversion techniques.

ESR 14 uses hyperparameters in a Bayesian hierarchical model to deal with structural uncertainty. It was found that by using features of the data (i.e. applying dimension reduction techniques), parts of the information contained in the data related to these hyperparameters can be selected. They made a comparison of different types of features to see which of them are the most effective in updating the posterior probability distribution of the structural parameters. They considered structural parameters that are either discrete (e.g. different geological scenarios or training images in multiple-point statistics simulations) and continuous (e.g. preferential orientation of channels).

ESR15 is developing a joint inversion procedure to couple time-lapse geophysical information (geoelectric and distributed temperature sensing) with time-lapse pressure and chemical concentration data. This methodology is being developed in the context of the seawater intrusion, so that density-dependent flow and solute transport must be coupled with soil electrical conductivity and soil temperature. The innovation of the procedure lies on the coupling of multiple physical process and on the introduction of geological constraints to the deterministic inverse problem.



3.4 Achieved and on-going activities, results and challenges

ESR 13 – Veronika Rieckh:

In the summer of 2018 a 3D combined salt/uranine tracer test was conducted in the test site of Lauswiesen (University of Tübingen, Germany). A complete set of 3D geoeletrical measurement of about 3500 quadripoles takes about 20 minutes and is repeated constantly. Except from direct sampling the whole setup works completely autronomous after tracer injection. As the amount of time series data is quite large, semi-automated filtering procedures are developed.

One of the main challenges is to develop a fast and accurate forward solver. Currently both a DUNE code (<u>https://www.dune-project.org/</u>) and a Matlab code are ready for use. Both are developed for solving the transient problem and modeling moments by using the moment generating equations. The difference of the codes lies within their speed, their flexibility and usability on a cluster and the accuracy. For the latter one, the moment generating equations for moments of electrical impedance for locations close to the source are often inaccurate.

- ESR 14 – Andrea Palacios

A time-lapse inversion was carried out with data from time-lapse cross-hole electrical resistivity tomography. The time-lapse results show that geophysical monitoring can image the seawater intrusion and can capture short-term and long-term conductivity, and thus, salinity variations. Long-term variations can be related to draught periods, whereas short-term variations relate to heavy rainfalls or storm surges.

Next steps include the choice of methodology for the integration of geological constraints to the inversion procedure and the coupling of the geoelectrical problem with the flow and transport problem.

- ESR 15 – Jorge López Alvis

Training in different methodological aspects was achieved: forward modeling of GPR traveltime, regularized inverse modeling, multivariate data analysis (principal component analysis, multidimensional scaling, kernel density estimation, k-means clustering, graphical probabilistic models). A proposed methodology to quantify structural uncertainty was validated and tested with a synthetic example of cross-borehole GPR traveltime data.

Results so far show that the proposed methodology is able to estimate uncertainty in structural parameters by considering prior geological information and geophysical data. Some challenges faced so far are related to the computational demand that may be required in case a complete inversion is desired and also to the high dimensionality of data space that is common when dealing with subsurface systems.



3.5 Added-value of the network

ENIGMA ITN gathers researchers from leading universities in Europe and North America and from private companies developing state-of-the-art technologies. The possibility for the ESRs to learn directly from these researchers in a professional, but friendly environment benefits them greatly. These exchanges occur during project meetings and during workshops every six months, so the ESRs have the opportunity to present their advances and challenges and to ask for counseling. As a network, research can be focused in issues that are important to the whole research community, and not only to a few individuals.

The secondments, time that an ESR spends in a partner university or company, also promote this collaboration with other experts. Plus, it teaches them to adapt to other countries, research groups and work environments. For example, ESR13 will do a secondment to focus on stochastic data inversion in Liège, from January until March 2019, enabling close collaboration opportunities appear with ESR 15 and Prof. Fréderic Nguyen; and, ESR14 will spend a few months in the University of Copenhagen to do joint experiments with ESR 7 at the Holtum site, under the supervision of Dr. Majken Looms and Prof. Peter Engesgaard. It is also planned to test the inverse modeling setup developed by ESR13, ESR14 and ESR15 with data from the Argentona site, during a secondment period that will take place at CSIC, in Barcelona, Spain.

Within the network, the ESRs 13, 14 and 15, working towards the same objective with different approaches, can meet, share ideas and share and discuss datasets in a much simpler manner. The different techniques developed by the ESRs can be compared, and group efforts can be made to take these results, discussions and conclusions to the scientific community through publications.

3.6 Dissemination activities

- ESR 13 – Veronika Rieckh:

April 2018: <u>Poster</u> presented during conference "Integrated Hydrosystem Modelling 2018", in Tübingen. July 2018: Poster presented during the 4th Cargèse Summer School, titled "<u>Fully-coupled Salt Tracer</u> <u>Test Tomography with Time-lapse Electrical Resistivity Tomography"</u>.

April 2019: Planned contribution at the European General Assembly (EGU) 2019.

ESR 14 – Andrea Palacios

June 2018: Oral presentation at the 25th Salt Water Intrusion Meeting (SWIM), titled "Time-lapse crosshole electrical resistivity tomography (CHERT) for monitoring seawater intrusion dynamics in a Mediterranean aquifer".

July 2018: Poster presented during the 4th Cargèse Summer School, titled "<u>Time-lapse cross-hole</u> <u>electrical resistivity tomography (CHERT) for monitoring seawater intrusion dynamics in a</u> <u>Mediterranean aquifer</u>"

December 2018: Oral presentation at the American Geophysical Union (AGU) 2018 Fall Meeting, in the Oral.

- ESR 15 – Jorge López Alvis

June 2018: Oral presentation at the 2018 Computational Methods in Water Resources (CMWR) conference, titled "Updating prior geologic uncertainty with GPR traveltime tomographic data".

July 2018: Poster presented during the 4th Cargèse Summer School, titled "<u>Updating uncertainty in</u> <u>hierarchical subsurface model using geophysical data: synthetic case for crossborehole-hole GPR</u>".



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