

Three-dimensional Multi-Scale and Multi-Method Inversion to Determine the Electrical Conductivity Distribution of the Subsurface Using Parallel Computing Architectures (Multi-EM)

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1. Objectives

Geophysical methods are applied to investigate the Earth's interior. We obtain models of the Earth by imaging physical parameters such as density, electrical conductivity, or elastic properties using a range of techniques. Here, we consider geophysical techniques exploiting natural and controlled-source electromagnetic (EM) fields to reconstruct the electrical conductivity structure at depth. During the last years, these techniques have experienced rapid development for exploration purposes of the drillable subsurface. For instance, active controlled-source electromagnetic (CSEM) techniques are now frequently used together with seismic techniques to characterize resistive hydrocarbon reservoirs in offshore petroleum exploration. Deep saline aquifers exhibit high electrical conductivities and constitute one of the prime targets for electrical imaging methods, making these techniques one of the most important geophysical tools to characterize target horizons for CO₂ storage or geothermal reservoirs.

In this project, we attempt to optimize the resolution capabilities of geoelectric potential

field and electromagnetic diffusion methods covering a wide range of scales from boreholes to regional or lithosphere dimensions. To reach these goals, we pursue an inter-disciplinary concept, integrating research groups from applied and numerical geophysics, information technology and numerical mathematics. The project partners come from university and non-university research institutions.

For tomographic imaging of a single physical parameter, the electrical conductivity, a number of well-proven techniques are available. In this project, we combine geoelectric methods (direct current - DC), transient electromagnetics (TEM), natural-source magnetotellurics (MT) and controlled-source magnetotellurics (CSMT) (see Fig. 1). The resolution power of the individual methods depends on the experimental design, the strength, geometry, and frequency content of the source fields and the characteristics of the induced current systems. Multi-scale, multi-method inversion strategies yield complementary but usually higher sensitivities when compared with existing inversions of the individual methods. Hence, a combina-

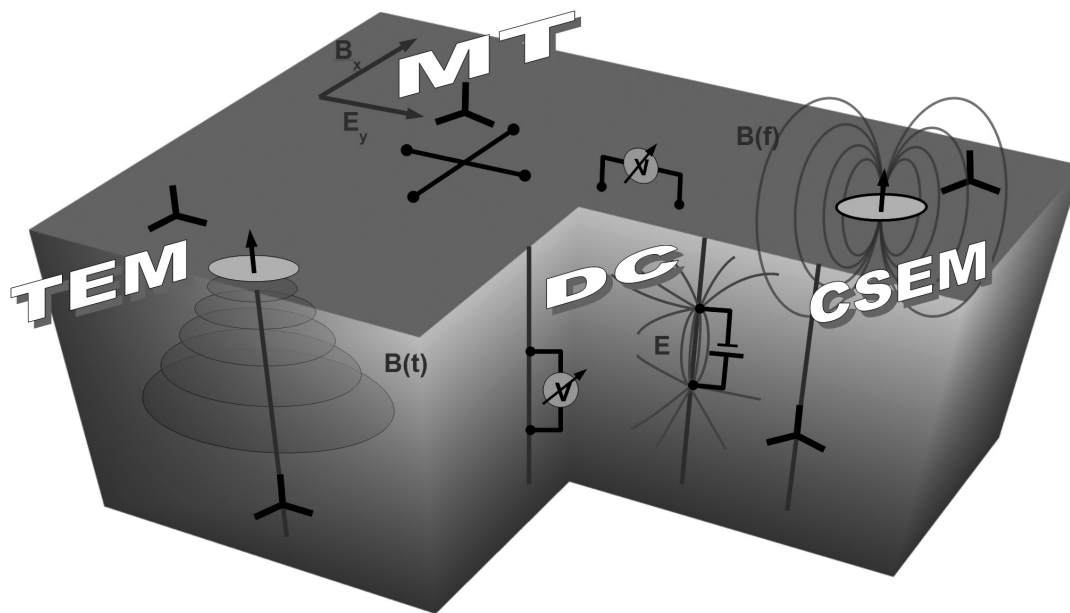


Figure 1: A combination of four electric and electromagnetic methods to enhance the reconstruction of the subsurface conductivity structure. Transient electromagnetics (TEM), DC resistivity, controlled-source electromagnetics (CSEM) and natural-source magnetotellurics (MT) cover a wide range of spatial scale lengths and provide individual and complementary sensitivity patterns.

tion of the various sensitivity patterns is expected to result in

- a better coverage of the model space
- a more complete and better resolved reconstruction of the conductivity structure
- a reduction of model ambiguities.

An effective implementation of multi-method, single-parameter inversions is a prerequisite for subsequent development of multi-method, multi-parameter inversions (e.g. a joint inversion of MT and seismic).

Realistic predictions of structures and materials at depth require three-dimensional modelling. The underlying differential equations can only be solved with numerical approaches, usually using finite difference (FD), finite element (FE) or integral equation (IE) techniques. The subsurface and the physical fields are discretized on grids, which in the three-dimensional domain easily consist of millions of individual

cells. The number of these grid cells and associated computations determines the requirements for memory and CPU time. However, a comprehensive image of the subsurface is only obtained with sufficiently fine discretization on a correspondingly large mesh. Solving these complex equation systems requires extremely powerful computers and highly optimized algorithms, which are often beyond the realms of individual working groups.

Considering the enormous numerical complexity of “normal” single-method three-dimensional inversions, the new algorithms will be designed from the beginning for massively parallel computing architectures. Initially, local computer clusters will serve as development environments, but integration with D-GRID or similar international structures is envisaged. The overall goal is to transfer the newly gathered knowledge and infrastructure to the wider geosciences community.

2. Introduction

The inversion of an electromagnetic data set to determine the electrical conductivity structure of the subsurface requires numerical methods. In three dimensions and for practically relevant models, several tens of thousands of data and model parameters are involved. Presently, such computationally intensive problems require high performance or supercomputers. Börner (2010) and Avdeev (2005) review state of the art three-dimensional electromagnetic numerical simulation and inversion strategies.

FD methods simulating the diffusion of transient fields in three-dimensional structures were first developed in the late 1980s (Newman et al., 1986). Wang and Hohmann (1993) introduced a time-stepping approach to compute the electromagnetic fields on a staggered grid (Finite Differences in the Time Domain, FDTD). The FDTD method is attractive because explicit time-stepping methods avoid solving linear equation systems. Commer and Newman (2004) demonstrated a numerical solution of the FDTD method on parallel computers.

A different approach to solving the TEM forward problem was presented by Druskin and Knizhnerman (1994), who introduced the spectral Lanczos decomposition method (SLDM). Here, Maxwell's equations are approximated on an FD grid, which leads to a system of ordinary differential equations. The solution of this system is reduced to the products of functionals of the stiffness matrix and a vector containing the initial conditions. Börner et al. (2008) developed the method of model reductions in the frequency domain (MRFD), which extends the SLDM method by combining it with the advantages of the FE methods on unstructured grids.

Adaptive grids with local refinements have predominantly been applied for FE methods (e.g. Franke et al. 2007; Rucker et al, 2006, Li and Key, 2007, Schwarzbach, 2009). For all of these methods the subsurface is subdivided into a large number of homogeneous cells organized

in ordinary or staggered grids (Yee, 1966) for which Maxwell's equations are solved.

Over the last few years, approaches to solve the 3D inverse problem have been suggested based on Newton, Quasi-Newton-, Gauss-Newton and non-linear conjugate gradient methods (Rodi and Mackie, 2001; Newman and Boggs, 2004; Commer and Newman, 2008, Avdeev and Avdeeva, 2009). All-at-once approaches attempt to solve the forward and the inverse problem simultaneously, applying an approximation to the forward solution (Haber et al., 2004). If the amount of data is less than the amount of model parameters, transformation to the data space can be advantageous (Siripunvaraporn and Egbert, 2005). Most inversion procedures are based on Gauss-Newton approaches using various forms of regularization (Smith and Booker, 1991; Oldenburg and Ellis, 1991; Sasaki, 2001; Günther et al., 2006). Often, the objective function represents a trade-off between optimum data fit and minimum structure of the model based on some smoothness constraint (de Groot-Hedlin and Constable, 1990). Newton techniques have favourable convergence characteristics, but require computationally costly second order derivatives of the objective function or derivatives of the sensitivities with respect to the model parameters.

Previous attempts to fit electromagnetic observations by 3D inversion include Patro and Egbert (2008) for magnetotelluric, Haber et al. (2007) for TEM, and Newman et al. (2010) for CSEM data. Commer and Newman (2009) consider the joint inversion of MT and CSEM data.

3. Work plan

Multi-method inversions of geoelectric and electromagnetic data require optimized and parallelized algorithms for the forward simulation which have to be well adapted to the specific resolution and model regularization of a particular method. The efficiency and suitable parallelization strategies for forward ope-

rators depend on the particular electrical or electromagnetic method. Inversion strategies, in contrast, can be developed largely independently of the individual methods. Nevertheless, multi-scale, multi-method inversions depend strongly on the regularization and model resolution of the individual methods. We therefore divide our work packages into tasks that can be addressed separately before being merged in a second step.

Multi-scales are introduced by different spatial resolution capabilities of the methods under consideration. Borehole tomography, for instance, can image the direct vicinity of a well at very high resolution, whereas MT measurements conducted at the surface of the Earth

cannot provide additional information at this scale. Conversely, well-logging cannot reveal structures of the subsurface at larger distances from the borehole. When combining both methods, the overlapping resolution domain is small and the multi-scale information content of the data is large. A common model that is consistent for both methods will be resolved in separate regions at dissimilar scales depending on the individual methods. The expression of the transition between resolved model domains and their inherent scales in the final model depends strongly on the regularization.

MT and CSMT are frequency domain methods using virtually identical sensor technology and similar survey geometry. Whereas passive MT

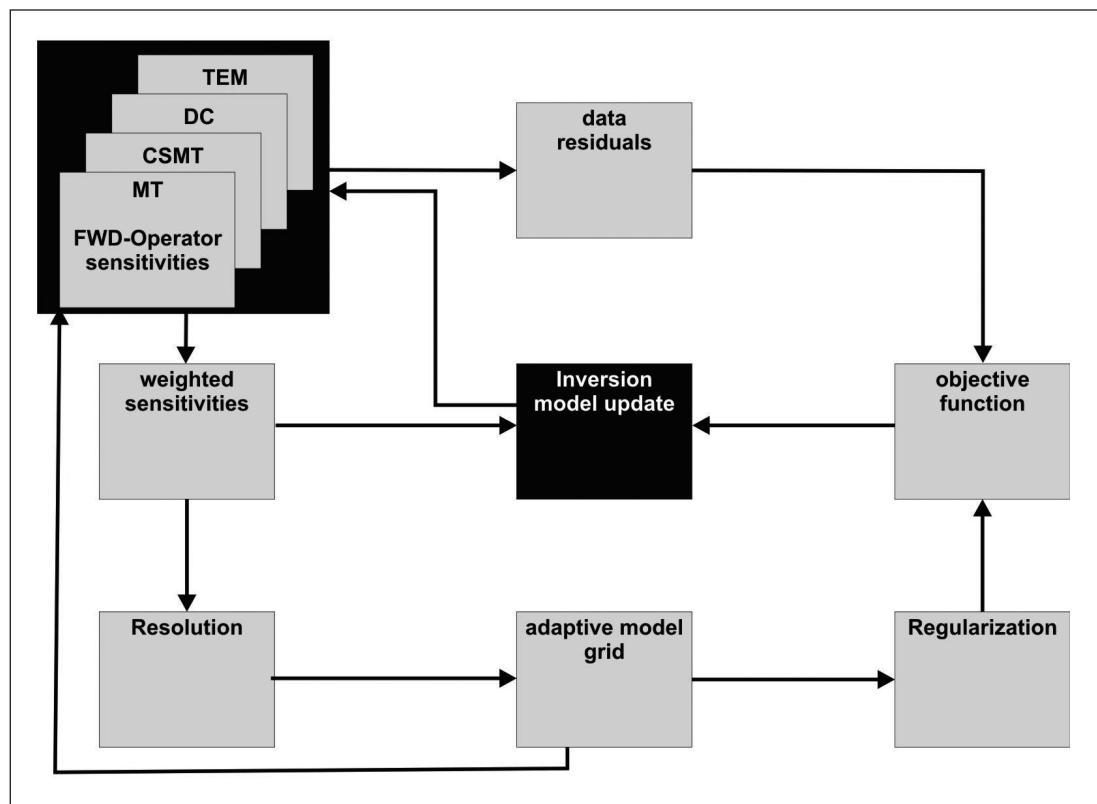


Figure 2: Flow chart of a multi-scale, joint EM inversion. In non-linear inversion, an objective function is defined, representing a measure of the distance between measured and synthetic data (i.e., data residuals). Synthetic data and data residuals are computed by applying a forward operator to a parameter model. Generally, the objective function is extended by a regularization term, which stabilizes the system and limits the solution space more or less arbitrarily. For joint inversion, we have to consider additional issues related to combining the methods. These include different resolutions (handled by using weighted sensitivities), optimized model discretizations (adaptive grids), and appropriate regularization techniques.

sources are usually assumed to be plane waves, in processing CSMT data, the geometry of the source and the near-field characteristics of the excited EM fields have to be considered. CSMT and classical MT have overlapping resolution domains on similar spatial scales. However, their sensitivities with respect to conductivity structures differ and are partly complementary. Due to the excitation of different current systems in the subsurface in MT and CSMT, MT has a high resolution potential for lateral conductivity variations, whereas CSMT has a comparatively better vertical resolution power for horizontal layering and for poor conductors. A combination of both methods by joint inversion should therefore be well-suited to increase the overall resolution beyond that of the individual methods, independently of the applied regularizations (Commer and Newman, 2009).

In subproject I (see below) the GFZ Potsdam group concentrates on the above mentioned combination of MT und CSMT. First, a 3D joint inversion of “normal” surface MT and CSMT data shall be developed (WP 1.02 – 1.04). Subsequently, this inversion will be extended by introducing resolution- and scale-dependent regularization strategies (WP 1.05) to facilitate, e.g., an integration of borehole data.

The main focus of the Freiberg working group is the combination of transient electromagnetics (TEM) and the DC resistivity method in subproject II. In WP 2.1 and WP 2.2 the specific sensitivity patterns of the individual methods are combined to enhance the resolution power for a given target area (WP 2.6). Both, DC resistivity and TEM can be applied from the surface or within boreholes. Using sensitivity and resolution analyses (WP 2.4, WP 2.5), optimum transmitter/receiver configurations can be determined to optimize experimental designs. In the mathematical part of WP 2.3, procedures will be developed to increase the efficiency of the geophysical interpretation techniques. Particularly, we will address model reduction in the frequency domain (MRFD), the spectral Lanczos decomposition method including re-

starts, so called thick restarts, rational Lanczos methods, and multigrid techniques.

The enormous complexity of three-dimensional inversions calls for the use of massively parallel computing architectures. In addition to the parallelization of numerical algorithms (WP 1.03, 1.09), this requires the development of scheduling algorithms to coordinate the execution of computing jobs in a distributed computing environment (WP 1.10). Job scheduling is particularly important when grid architectures are used as a computing resource (Fernandez-Quiruelas et al., 2009).

Subproject 1:
Joint inversion of CSMT and MT, implementation of concepts for distributed computing.

WP 1.01
Benchmarking of various existing 3D MT and 3D CSMT forward and inversion codes.

WP 1.02
Extension of a 3D code for joint inversion of CSMT und MT:

The development of the joint inversion will combine the modular, open source code from Egbert (Egbert et al., pers. communication), which presently includes a range of options for MT modelling and more generally applicable inversion schemes, with existing CSEM modelling codes (Streich, 2009; Streich and Becken, 2011). In addition, optimized strategies for regularization and design of the inversion meshes for a joint CSMT and MT inversion must be defined, considering the different and complementary sensitivities of the two methods (WP 1.04). Furthermore, global weighting of the individual methods as described by Commer and Newman (2009) can be used.

WP 1.03
Efficient parallelization of implemented algorithms:

We will develop and implement parallelization

strategies that are specific to each individual method. For instance, when using iterative solvers, the MT forward problem can be computed in parallel for each period and polarisation, and the sensitivity matrix can be computed for all receivers autonomously. We will also utilize parallelized direct solvers, initially for CSEM modelling and inversion. Direct solution approaches are memory-intensive, but advantageous if solutions for many sources and sensitivities for many receivers are required. Inversion techniques which so far have been considered impractical because of the large number of forward modelling solutions required may thus become feasible. In addition to these different levels of parallelization within our modelling and inversion algorithms, we shall also use and possibly adapt parallelized algorithms for matrix operations, such as PETSc, PSBLAS or ScaLAPACK (see also WP 1.09 and 1.10).

WP 1.04

Multi-grid methods and adaptive meshes for multi-scale problems:

Scaling properties of CSMT and MT models may be comparable, but the spatial behaviour of the associated electromagnetic fields differs significantly between the two methods. Whereas the external magnetic source fields in MT can be treated as quasi-homogenous plane waves, the source fields and secondary currents in the vicinity of a CSMT transmitter are extremely heterogeneous and exhibit strong gradients. Consequently, numerical CSMT simulations generally require much finer meshes than MT simulations, and local mesh refinements near the source can be advantageous for CSMT simulations. To generate optimized meshes that permit accurate computations of EM fields using as few cells as possible but as many as necessary, adaptive methods for grid refinement shall be applied in the forward computations. Similarly, for the inversion, we will develop adaptive methods that adjust the mesh according to the model sensitivities. Adaptive inversion meshes will also be used in the multi-scale inversion of combined borehole and surface measurements (see also WP 1.05).

WP 1.05

Optimisation of regularisation schemes:

All electrical and electromagnetic inverse problems are ill-posed and require regularization. Common regularization schemes impose smoothness constraints on the electrical conductivity structure. The solution is then determined as a trade-off between the model norm (or an a priori defined semi-norm) and the data residuals. Usually, model structure is penalized with a (weighted) global constraint, which may lead to over-regularisation of well resolved model domains and under-regularization of badly resolved regions. Such global penalties are inappropriate for multi-scale inversion algorithms. We therefore aim to develop a posteriori regularization strategies that depend on the model resolution on a local scale, possibly making use of strategies similar to Scherzer et al., 1993; Kaltenbacher and Schicho, 2002; Raus and Hämarik, 2009, which are not yet widely used for EM inversion.

In multi-grid approaches, a resolution-dependent regularization can be found by discretizing the model space depending on the resolution and defining the regularization operator in the model space: Well-resolved model regions are finely discretized and thus require little regularization. Kaltenbacher and Schicho (2002) show that such an approach converges for ill-posed non-linear problems. In this work package, we attempt to develop an implicit local regularization by adaptive model parameter discretization for multi-scale problems, such as the joint inversion of surface and borehole data. This first requires testing strategies for adaptive model refinement (see also WP 1.04).

WP 1.06

Wavelet parameterisation:

To reduce the number of degrees of freedom in the model and the associated size of the inverse problem, the model parameters can also be represented in the wavelet domain. A major challenge in using wavelet parameterisation is identifying the significance of coefficients, as predicting the significance of coefficients for

the next iteration will be necessary when solving nonlinear equation systems iteratively. For an efficient inversion, these predictions must be achieved without explicitly computing the wavelet coefficients. To this end, we attempt to transfer methods for adaptive model discretization of WP 1.04 to the wavelet domain.

WP 1.07

Application to existing field data:

The newly developed inversion schemes will be applied to and tested with existing field data. MT data sets with areal site coverage that are suitable for 3D inversion are available from various projects (Namibia, South Africa, Dead Sea Transform, San Andreas Fault, North-German basin, Groß Schönebeck). Within the ongoing GeoEn project, the GFZ working group has acquired a large CSMT data set in the vicinity of the CO₂ sequestration test site near Ketzin. Since MT data were also collected in the same survey, these data may be used for testing the multi-scale joint inversion.

WP 1.08

Communication Platform:

Implementation of a web-based communication platform that will serve as a tool for an exchange of experiences, to publish best practice guides, and to document project and administrative matters. The platform will be available throughout the project and after the project has ended.

WP 1.09

Implementation of parallel computing and open source packages on the compute cluster:

For the development of parallel algorithms, several Message Passing Interface (MPI) software packages, which are capable of using the infiniband network, and compatible Fortran and C compilers (Intel, Portland, GNU) are installed on the GFZ computer cluster. In this work package we will investigate the combination of distributed memory, MPI-based and shared-memory (OpenMP) parallelization that can be used within multi-core cluster nodes.

WP 1.10

Development of scheduling algorithms for distributed computing:

In addition to the compute cluster of the GFZ, the project aims to facilitate the use of Grid computing technologies, such as the D-GRID network (Klump and Häner, 2005). Besides parallelization of algorithms, the distributed nature of the Grid requires development of scheduling algorithms to orchestrate distributed compute jobs dispatched to remote Grid computing nodes. The Grid resources will be made accessible through a web portal. The results of this work package will be disseminated to the project partners and a wider user community via the workshops and the project communication platform (WP 1.08). A longer-term goal of this work package is to facilitate access to the compute and storage resources of the Grid for the geosciences community to provide computing resources which are well beyond the current means of individual research groups. We have initiated discussions to coordinate these efforts with the BMBF-funded WissGrid project.

Sub-project 2:

Joint inversion of transient electromagnetic and DC resistivity methods

WP 2.01

Further development and parallelization of forward modelling operators for DC resistivity methods: (see WP 2.02).

WP 2.02

Further development and parallelization of forward modelling operators for transient electromagnetic (TEM): The working group in Freiberg have developed their own, fast forward operators for DC electrics (Rücker et al., 2006) and TEM (Börner et al., 2008). Both codes use an unstructured grid finite element approach (Lagrange type for DC resistivity and Nédélec type for TEM), such that given structures can be transferred to synthetic models in great detail. These codes are powerful tools for practical use. Within this work package we want to

assess if the originally sequentially structured codes can be parallelized or have to be reengineered to facilitate efficient parallelization.

WP 2.03

Further development of the spectral Lanczos method: The interpretation software for TEM data, which has been developed during the last three years within the DFG project 'Numerical simulation of the propagation of transient electromagnetic fields for the exploration of the subsurface', is based on the finite element discretization of the three-dimensional quasi-static Maxwell's equations in space (Nédélec elements) and the solution of the semi-discrete problem by advancing the spectral Lanczos decomposition method (SLDM) using restarts (Eiermann and Ernst, 2006). Restarted algorithms reduce the memory requirement of SLDM significantly (or supersede a second run of the Lanczos algorithm, respectively). However, they converge generally slower than the variant without restarts. Another newly developed approach called 'thick restarts' may compensate the loss of speed without waiving the advantages of restarts. This technique will further accelerate our forward solver. In recent years, so called rational Lanczos methods were investigated at the Institute of Numerical Analysis and Optimization as an alternative to the classical Lanczos method. The crucial advantage of this method is the fact that its convergence rate does not depend on the size of the problem (at least for the problems at hand). Whereas classical SLDM needs additional iteration steps with increasing resolution to reach a given accuracy level, the number of iterations remains constant for the rational Lanczos method – an important advantage for the solution of very large problems. Since for the rational Lanczos method one linear system of equations of the type $(A - \lambda I)x = b$ has to be solved in each iteration step with A being the discrete version of Maxwell's equations and possibly including a complex shift λ , fast solvers are an essential prerequisite for the application of these methods. Therefore, we need to apply multi-grid methods that are specifically deve-

loped for the curl-curl operator and have been shown to exhibit robust convergence rates with respect to the choice of the shifts.

WP 2.04

DC resistivity method:

resolution analyses, optimization of the experimental design (see WP 2.05).

WP 2.05

TEM: resolution analyses, optimization of the experimental design:

Apart from the actual simulation, the computation of sensitivities is complicated and numerically very costly. Günther et al. (2006) und Baranwal et al. (2007) have developed working inversion codes which have increased our knowledge about resolution characteristics of the DC and TEM methods (see also Spitzer, 1998). For both applications, we employ adjoint field techniques, which have partly been implemented (Ullmann, 2008), but require further development and adaptation to large and powerful computers. The envisaged modular, flawless inversion code would simplify an efficient parallelization. By means of a joint DC/TEM inversion we can investigate the resolution characteristics of different experimental designs in order to optimize the resolution power of field experiments. In other words, we intend to develop a tool telling us where to place receivers and sources to obtain an optimal (with the highest resolution) image of the target structures (see Stummer et al., 2004).

WP 2.06

Combination of both methods in a joint inversion:

After developing the individual inversion algorithms for TEM and DC, we will start implementing a joint inversion scheme. In this context, problems with the combined parameterizations have to be solved. By means of sensitivities we can compute resolution matrices to assess the resolution characteristics of the individual methods and subsequently of their combination. Common sub-project III: Synthesis, knowledge transfer and publications

WP 3.01

Definition of interfaces:

For combining the modules developed in sub-projects I and II, suitable interfaces have to be defined and incorporated into the developed codes. The interfaces will initially be defined in the workshops at project commencement. Necessary extensions and adjustments will then be agreed upon during consecutive workshops (WP 3.03) and using the communication platform (WP 3.04).

WP 3.02

Synthesis of DC, TEM, MT and CSMT:

Questions concerning parameterization, modularization, implementation and parallelization of the individual methods and eventually their combination will be examined in close cooperation between all working groups of sub-projects I and II. Once the separate inversions are running, they will be combined into a common joint inversion scheme. All working groups will be involved in this task.

WP 3.03

Workshops:

Part and parcel of this cooperation are regularly held workshops where project partners and their associated working groups meet. These workshops will be held every 6 months, alternating between Freiberg and Potsdam. The workshops participants will report on the status of the ongoing work, develop common inversion strategies, and use synergies to parallelize and implement inversion codes.

WP 3.04

Information platform:

In addition to the workshops, communication between project partners will be supported by web-reporting and web-based tools (see WP 1.08). Information will be processed by project participants and made available to all partners.

WP 3.05

Scientific results obtained within this project will be presented at national and international conferences and published in international, peer-reviewed journals.

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