A PENALTY METHOD FOR PDE-CONSTRAINED OPTIMIZATION

FIELD OF THE INVENTION

5   The invention relates to a partial-differential-equation (PDE) constrained optimization method and especially to a partial-differential-equation (PDE) constrained optimization method for geophysical prospecting.

BACKGROUND OF THE INVENTION

10   Partial-differential-equation (PDE) based inversion methods aim to find estimates of unknown physical model parameters. For example in geophysical prospecting compressional wavespeeds from partial measurements of a subsurface formation is used. By finding solutions of a partial differential equation which best explain the observed data subject to constraints imposed by e.g. the physics and the

15   geology one can obtain a model. The model can be used to image the subsurface formation and provide valuable information regarding for example the presence of oil or gas reserves.

          There exists a wide body of literature on these methods that fall into one or more of the following categories:

20   -   PDE-constrained optimization formulations (hereafter referred to as the constrained formulation) where the data misfit is minimized subject to PDE constraints (Eldad Haber, Ascher, and Oldenburg 2000). Solutions of the PDE and physical model parameters are simultaneously updated in these approaches that involve the solution of large sparse systems of

25   equations also known as KKT systems. Because this method updates the physical model parameters as well as the forward and adjoint fields at each iteration, it requires concurrent access to these fields for all sources, i.e., right-hand sides of the PDE. This leads to infeasible demands on storage for large-scale applications, such as 3D seismic inversion, which

consists of many source experiments with a large number of measurements.

- Unconstrained or reduced formulations as described by Haber, Eldad, Uri M. Ascher, and Doug Oldenburg. 2000. "On optimization techniques for solving nonlinear inverse problems." *Inverse Problems* 16 (5) (oct): 1263–1280. doi:10.1088/0266-5611/16/5/309 are hereafter referred to as the reduced formulation. In the reduced formulation the PDE constraint is eliminated by solving the PDE. This method requires for each iteration solutions of the forward and adjoint systems as explained by Tarantola, A., and A. Valette. 1982. "Generalized nonlinear inverse problems solved using the least squares criterion." *Reviews of Geophysics and Space Physics* 20 (2): 129–232 and by Plessix, R.-E. 2006. "A review of the adjoint-state method for computing the gradient of a functional with geophysical applications." *Geophysical Journal International* 167 (2): 495–503. As opposed to the constrained formulations, the Jacobian and (Gauss-Newton) Hessian are dense and their application requires additional PDE solves. However, the gradients and Hessian are built up source by source and do not require storage of the fields for all sources for each model update making this a practical method for large/complex industrial applications.

- The equation-error approach as described by Richter, R. G. 1981. "Numerical Identification of a Spatially Varying Diffusion Coefficient." *Mathematics of Computation* 36 (154): 375–386, which requires complete measurements of the field in the region of interest and uses the PDE, the source terms and the measured field to setup a system of (non)linear equations for the physical model parameters.

- Iterative fixed-point series methods as described by Weglein, Arthur B., Fernanda V. Araújo, Paulo M. Carvalho, Robert H. Stolt, Kenneth H. Matson, Richard T. Coates, Dennis Corrigan, Douglas J. Foster, Simon A. Shaw, and Haiyan Zhang. 2003. "Inverse scattering series and seismic exploration." *Inverse Problems* 19 (6) (dec): R27–R83. doi:10.1088/0266-

5611/19/6/R01, during which physical model parameters are estimated by expanding the forward model into a series with different order contributions. Iterations in this case, correspond to including higher order terms in the expansion.

- Iterative fixed-point contrast-source formulation as described by van den Berg, P. M., and R. E. Kleinman. 1997. "A contrast source inversion method." *Inverse Problems* 13 (6): 1620–1706, which involves alternating solves for sources and contrasts from the Lippmann-Schwinger equation and the data equations.

- Linearized inversions as described by Plessix, R.-E., and W. A. Mulder. 2004. "Frequency-domain finite-difference amplitude-preserving migration." *Geophysical Journal International* 157: 975–987, during which the initial simple physical model parameters with respect to which the linearization has been carried out are not updated. These methods correspond to a single gradient or Gauss-Newton step. These linearized algorithms minimize the mismatch between a fixed data residual and the linearized forward model using local derivative information. In cases where the initial simple physical model parameters are far from their true values, these linearized approaches do generally not lead to accurate estimates for the perturbation of physical model parameters with respect the initial physical model.

- Iterative global nonlinear inversions as described by Tarantola, Albert. 2005. *Inverse problem theory and methods for model parameter estimation*. Society for Industrial Mathematics, during which the physical model parameters are estimated by means of a global search amongst all possible parameter combinations that best explain the observed data according to some data-misfit functional. Examples of these methods include Monte-Carlo methods, genetic algorithms, and simulated annealing. The costs of PDE solves are generally too high to warrant these approaches viable for physical models with high-dimensional parameterizations.

The two most widely used and practical methods for large-scale problems are the constrained and reduced formulations, both of which have their advantages and disadvantages.

An advantage of the constrained formulation is that the forward and adjoint PDEs never need to be solved explicitly, as the forward and adjoint fields are updated simultaneously with the physical model parameters. A further advantage is that the search space for the optimization is much bigger than for the reduced method, possibly mitigating some of the problems that are ubiquitous in the reduced formulation such as local minima. A disadvantage of the constrained formulation is that it requires storing and updating of all fields.

An advantage of the reduced formulation is that the PDEs for all right-hand sides can be solved independently (and possibly in parallel) and the results can be aggregated in a running sum making the method applicable for large/complex industrial applications. Further the reduced formulation allows for integration into black-box nonlinear optimization schemed that only require misfit and derivative information such as the gradient. Disadvantages of the reduced formulation are that the PDEs need to be solved explicitly at each iteration and that the Jacobian and Hessian are dense and can only be applied in a matrix-free sense each requiring PDE solves. Furthermore because the PDE is eliminated, the search space for the optimization is reduced to the physical model parameters only, making the method more prone to get trapped in local minima.

When a partial-differential-equation constrained optimization method is used for geophysical prospecting of areas having a large geological complexity, simple background physical parameter models are usually unavailable. An iterative local nonlinear inversion based on the reduced formulation, known as full-waveform inversion (FWI), is then usually the method of choice. Practical application of this methodology is however hampered by:

- excessive computational and memory-storage costs exacerbated by the fact that these methods require several iterations that involve PDE solves. Dimensionality reduction techniques as described in WO2011160201 and by Haber, Eldad, Matthias Chung, and Felix Herrmann. 2012. "An

Effective Method for Parameter Estimation with PDE Constraints with Multiple Right-Hand Sides." SIAM Journal on Optimization 22 (3) (jul): 739–757. doi:10.1137/11081126X can be used to bring these costs down. Dimensionality-reduction techniques include batching as described by

5   Aravkin, Aleksandr, Michael P. Friedlander, Felix J. Herrmann, and Tristan Leeuwen. 2012. "Robust inversion, dimensionality reduction, and randomized sampling." Mathematical Programming 134 (1) (jun): 101–125. doi:10.1007/s10107-012-0571-6 and Gauss-Newton with compressive sensing as described by Li, X., A. Y. Aravkin, T. van Leeuwen,

10   and F. J. Herrmann. 2012. "Fast randomized full-waveform inversion with compressive sensing." Geophysics 77 (3): A13. doi:10.1190/geo2011-0410.1, reduce the computational burden of FWI significantly, these methods require additional solutions of the forward and adjoint wave equations.

15   -   local minima caused by cycle skipping, which occur when the kinematics of the predicted data for the current estimate of the physical model parameters differs by more than half a wavelength compared to the kinematics of the corresponding event in the observed data. Numerous techniques have been developed to mitigate this detrimental effect

20   including (a) multiscale continuation methods where the inversions for the physical parameters are carried out by starting at the long wavelengths and using these parameter estimates as warm starts for inversions at the shorter wavelengths (Bunks, Carey. 1995. "Multiscale seismic waveform inversion." Geophysics 60 (5) (sep): 1457.

25   doi:10.1190/1.1443880) and (b) offset and Laplace parameter continuations where the inversions for the physical parameters are carried out by starting at the small offsets and short time windows after the first arrival and using these parameter estimates as warm starts for inversions at larger offsets and over longer time windows (smaller

30   Laplace parameters) (Pratt, G. R., Changsoo Shin, and G. J. Hicks. 1998. "Gauss-Newton and full Newton methods in frequency-space seismic

waveform inversion." Geophysical Journal International 133 (2) (may): 341–362. doi:10.1046/j.1365-246X.1998.00498.x and Brossier, Romain, Stéphane Operto, and Jean Virieux. 2009. "Seismic imaging of complex onshore structures by 2D elastic frequency-domain full-waveform inversion." GEOPHYSICS 74 (6) (nov): WCC105–WCC118. doi:10.1190/1.3215771). While the above solutions have been applied successfully, the effectiveness of these methods in practice is somewhat limited because of missing low frequencies, due to low signal-to-noise ratios at low frequencies and missing long offsets due to physical constraints such as finite cable lengths and cost considerations related to field-data acquisition.

The above may also be explained as follows. For PDEs where solutions are linearly related to the source function, PDE-constrained optimization takes the following mathematical form (E. Haber and Ascher 2001):

(1) $\quad min_{\mathbf{m},\mathbf{u}} \sum_{i=1}^{M} \frac{1}{2} \parallel P_i\mathbf{u}_i - \mathbf{d}_i \parallel_2^2 \quad$ s. t. $\quad A_i(\mathbf{m})\mathbf{u}_i = \mathbf{q}_i, \quad i = 1\cdots M,$

where

- $\mathbf{m} \in \mathbb{C}^N$ is a vector of length N with gridded medium parameters,
- $i = 1\cdots M$ is the experiment index with M the number of experiments,
- $\mathbf{d}_i \in \mathbb{C}^K$ are the observed data with K the number of samples,
- $A_i(\mathbf{m})$ is the system matrix,
- $\mathbf{q}_i \in \mathbb{C}^N$ represent the discretized source vectors,
- $\mathbf{u}_i \in \mathbb{C}^N$ are the corresponding discretized fields,
- P_i is the detection operator for the ith source experiment.

Such constrained optimization problems can be solved by the Lagrangian as in Haber, E., and U. M. Ascher. 2001. "Preconditioned all-at-once methods for large, sparse parameter estimation problems." *Inverse Problems* 17 (6) (dec): 1847–1864. doi:10.1088/0266-5611/17/6/319.

(2) $\quad L(\mathbf{m}, \mathbf{u}, \mathbf{v}) = \sum_{i=1}^{M} \frac{1}{2} \parallel P_i\mathbf{u}_i - \mathbf{d}_i \parallel_2^2 + \langle \mathbf{v}_i, A_i(\mathbf{m})\mathbf{u}_i - \mathbf{q}_i \rangle,$

where $\mathbf{u} = [\mathbf{u}_1; \cdots; \mathbf{u}_M]$ collects the wavefields for each source experiment and $\mathbf{v} = [\mathbf{v}_1; \cdots; \mathbf{v}_M]$ are the Lagrange multipliers for each source experiment. Solving this optimization problem with a Newton-like method leads to the KKT system:

$$\begin{pmatrix} * & * & G^* \\ * & P^*P +* & A^* \\ G & A & 0 \end{pmatrix} \begin{pmatrix} \delta\mathbf{m} \\ \delta\mathbf{u} \\ \delta\mathbf{v} \end{pmatrix} = -\begin{pmatrix} G^*\mathbf{v} \\ A^*\mathbf{v} + P^*(P\mathbf{u} - \mathbf{d}) \\ A\mathbf{u} - \mathbf{q} \end{pmatrix},$$

where $*$ denotes second-order terms, A (and its conjugate transpose or adjoint A^* is block diagonal matrix containing the matrices A_i and similarly for P and G, with

$$G_i(\mathbf{m}, \mathbf{u}) = \frac{\partial A_i(\mathbf{m})\mathbf{u}_i}{\partial \mathbf{m}}.$$

The basic iterative algorithm to solve the constrained formulation consists of the following steps:

1. select appropriate initial guesses, $\mathbf{m}^0, \mathbf{u}_i^0, \mathbf{v}_i^0$ for all i,

2. solve the KKT system to obtain updates $\delta\mathbf{m}, \delta\mathbf{u}_i, \delta\mathbf{v}_i$, for all the experiments i,

3. determine a steplength α,

4. update

$$\mathbf{m}^{k+1} = \mathbf{m}^k + \alpha\delta\mathbf{m}, \mathbf{u}_i^{k+1} = \mathbf{u}_i^k + \alpha\delta\mathbf{u}_i, \mathbf{v}_i^{k+1} = \mathbf{v}_i^k + \alpha\delta\mathbf{v}_i$$

for all i, and repeat steps 2-4 until a predetermined stopping criterion is met.

Because the method solves the forward and adjoint PDEs simultaneously, it eliminates the need to explicitly solve the forward and adjoint PDEs. The constrained formulation has the following advantages:

- as suggested by Asher and Haber (Ascher, Uri M., and Eldad Haber. 2005. "Computational Methods for Large Distributed Parameter Estimation Problems in 3D." In *Modeling, Simulation and Optimization of Complex Processes*, ed. HansGeorg Bock, HoangXuan Phu, Ekaterina Kostina, and Rolf Rannacher, 15–36. Springer Berlin Heidelberg) PDE-constrained formulations have the advantage that the PDEs do not need to be solved explicitly, and

- since constrained optimization methods search over a much larger solution space, there are reasons to believe that this formulation reduces the risk of the algorithm becoming trapped in a local minimum.

Unfortunately, constrained optimization methods are impractical for large-scale applications with many experiments (i.e., large M) because they need to store the forward and adjoint fields for each source. This means that each update requires access to all $2M$ fields, which prohibits its use for large-scale problems with many sources such as in the above referred to seismic applications.

The reduced formulation is based on the fact that it is found to be unfeasible to store and update all $2M$ fields as part of an iterative procedure (Epanomeritakis, I., V. Akçelik, O. Ghattas, and J. Bielak. 2008. "A Newton-CG method for large-scale three-dimensional elastic full-waveform seismic inversion." *Inverse Problems* 24 (3) (jun): 034015. doi:10.1088/0266-5611/24/3/034015). In view of this practical methods eliminate the PDE constraints in Equation (1), yielding the unconstrained or reduced formulation involving the minimization of the following misfit cost functional:

$$(3) \qquad min_{\mathbf{m}}\phi_{\mathrm{red}}(\mathbf{m}) = \sum_{i=1}^{M} \frac{1}{2} \parallel P_i A_i(\mathbf{m})^{-1}\mathbf{q}_i - \mathbf{d}_i \parallel_2^2.$$

The gradient of this objective is given by

$$\nabla\phi_{red}(\mathbf{m}) = \sum_{i=1}^{M} G_i\,(\mathbf{m}, \mathbf{u}_i)^*\mathbf{v}_i,$$

where

$$\begin{aligned} A_i(\mathbf{m})\mathbf{u}_i &= \mathbf{q}_i \\ A_i(\mathbf{m})^*\mathbf{v} &= -P_i^*(P_i\mathbf{u}_i - \mathbf{d}_i). \end{aligned}$$

The Gauss-Newton Hessian is given by

$$H_{GN} = \sum_{i=1}^{M} G_i^* A_i^{-*} P_i^T P_i A_i^{-1} G_i,$$

which is a dense matrix. In practice, this matrix is never stored but its action is computed via additional PDE solves.

The basic iterative algorithm to solve the reduced formulation consists of the following steps:

1. select an appropriate initial guess $\mathbf{m}^0$,

2. solve the forward PDEs $A_i(\mathbf{m}^k)\mathbf{u}_i = \mathbf{q}_i$ for all i,

3. solve the adjoint PDEs $A_i(\mathbf{m}^k)^*\mathbf{v} = -P_i^*(P_i\mathbf{u}_i - \mathbf{d}_i)$ for all i,

4. compute the gradient $\mathbf{g} = \sum_{i=1}^M G_i(\mathbf{m}^k, \mathbf{u}_i)^*\mathbf{v}_i$ by aggregating the results from steps 2,3 over all i,

5. scale the gradient, for example with the inverse of the GN Hessian $\delta\mathbf{m} = -H_{GN}^{-1}\nabla\phi_{red}(\mathbf{m})$,

6. determine a steplength α.

7. update $\mathbf{m}^{k+1} = \mathbf{m}^k + \alpha\delta\mathbf{m}$ and repeat steps 2-7 until a predetermined stopping criterion is met.

This reduced formulation requires explicit solves for the forward and adjoint PDEs to evaluate the objective and its gradient. Evaluation of the action of the Hessian requires additional PDE solves. However, the PDEs can be solved for all $i = 1\cdots M$ sources separately possibly in parallel and without the need to store all $2M$ fields at any time.

The aim of the present invention is to provide a partial-differential-equation (PDE) constrained optimization method, especially suited for geophysical prospecting, but not limited to geophysical prospecting, which does not have the above-described disadvantages of the constrained and reduced formulations. More especially a method is aimed at that is less likely to stall and capable to work with large data volumes with many sources.

SUMMARY OF THE INVENTION

This aim is achieved by the following method. A computer-implemented method for obtaining a physical model having physical model parameters wherein solutions to one or more partial-differential-equations (PDE's) are calculated, wherein the PDE's are constrained by observed data from a system whose response to a known source function and known sampling operator is modeled by solutions of those PDEs for a given physical model using physical model parameters, wherein (i) an appropriate initial model is selected, (ii) setup a system of equations referred

to as the data-augmented PDE for the field, comprising of the discretized PDE, the sampling operator, the source function and the observed data, and solve the data-augmented PDE in a suitable manner to obtain a field that both satisfies the PDE and fits the data to some degree, (iii) setup a system of equations by using the PDE, the source function and the field obtained in step (ii) and solve this system of equations in a suitable manner to obtain an update of the physical model parameters and repeat steps (ii)-(iii) until a predetermined stopping criterion is met.

Applicants found that compared to the known all-at-once approaches to PDE-constrained optimization as discussed above, there is no need to update and store the fields for all sources leading to significant memory savings when the method according to the invention is used. For example when the method is used to obtain a model of a geological area by means of wave-equation based inversion it has been found that the method is able to solve the full-waveform inversion problem without the necessity to form adjoint wavefields. The method further avoids local minima and thus is less likely to stall. Further advantages and applications of the method according to the invention will be described below.

Brief description of the drawings

Figure 1 is a schematic flow scheme of the method according to the invention.

Figure 2 is a flow scheme of a prior art FWI method.

Figure 3 is a flow scheme of a FWI method according to the invention.

Figure 4 shows an image representing the Square velocity perturbation embedded in constant background related to Example 1.

Figure 5 shows an image representing the Scattered wavefield for a point source corresponding to the model depicted in example1.

Figure 6 shows an image representing the Scattered wavefield obtained by solving for a constant velocity in Example 1.

Figure 7 shows an image representing the Estimate of model parameters in Example 1.

Fig. 8 shows an image representing the Velocity perturbation of Example 2.

Fig. 9 shows an image representing the Traditional reverse-time migration of Example 2.

Fig. 10 shows an image obtained by Example 2.

Fig. 11 shows an image representing the Misfit as a function of v_0 for the prior art and method according to the invention in Example 3.

Fig. 12 shows an image representing the Reconstructed velocity profiles after 1000 steepest descent iterations in Example 4.

Fig. 13 shows an image representing the Convergence histories in Example 4.

Fig. 14 shows an image representing the Data corresponding to the reconstructed velocity profiles in Example 4.

DETAILED DESCRIPTION OF EMBODIMENTS

In the method according to the invention the following terms are used:

Physical model: a model of a physical entity, wherein the physical entity is described by physical properties that appear in PDE's that describe the response of this physical entity to an external excitation expressed by a source function. The physical entity may be for example a geological area, the earth's subsurface, atmospheric conditions, the human body.

Physical model parameters: parameters used in the model to describe the physical entity.

Partial-differential-equations (PDE's): a set of equations that describes the field resulting from an external excitation. For example when an acoustic excitation is applied the field is the wavefield and the PDE is the wave equation.

Discretized PDE: a system of equations obtained by discretizing the PDE with the method of finite differences, finite elements or by any other appropriate discretization method as to model the solution of the PDE in a computer.

System matrix: This is the part of discretized PDE that acts on the discretized field and that contains the physical model parameters.

PDE residue or Wave equation residual: a vector expressing the difference between the action of the system matrix, containing the discretized physical model

parameters and spatio/temporal difference operators, on the field and the source function.

Field: solution of the PDE.

Source function: mathematical representation of the external excitation. A

5   source function may for example be an impulsive source located at the surface and represented by a vector with all zeros except for a (complex) number at the location that corresponds to the source.

Observed data: physical measurements that are taken of the response of the physical entity to the external excitation.

10   Sampling operator: a linear operator that models the physical process of taking measurements, also referred to as acquisition or detection operator.

Source experiment or the ith source experiment represents the, i^{th}, experiment generally with different source locations and/or different source functions.

15   The terms cheap or low costs is used to characterize a feasible method, which can handle large industrial problems, requiring less, i.e. cheap, computer capacity, The term expensive or high costs is used to characterize a not-feasible method, which cannot handle large industrial problems, which would require unrealistic large and expensive computer capacity.

20   The method according to the present invention is a computationally efficient method of solving partial-differential-equation (PDE)-constrained optimization problems that occur in (geophysical) inversion problems and/or in other fields of use as described in this application. The method takes measured data from a physical system as input and minimizes an objective function that depends on an

25   unknown model for the physical parameters, fields, and additional nuisance parameters. The objective function may be described by equation (4):

$$(4) \quad \phi_\lambda(\mathbf{m}, \mathbf{u}) = \sum_{i=1}^{M} \frac{1}{2} \parallel P_i \mathbf{u}_i - \mathbf{d}_i \parallel_2^2 + \frac{\lambda^2}{2} \parallel A_i(\mathbf{m})\mathbf{u}_i - \mathbf{q}_i \parallel_2^2.$$

parameterized by the physical model parameters **m**, wherein **m, u, d, q,** *M, i* , $A_i(\mathbf{m})$ and P_i have the same meaning as defined for equation (2) and wherein λ is

30   a trade-off parameter and wherein the least-squares data-misfit term,

$\| P_i\mathbf{u}_i - \mathbf{d}_i \|_2^2$, and the λ-weighted PDE-residual term, $\| A_i(\mathbf{m})\mathbf{u}_i - \mathbf{q}_i \|_2^2$, in equation (4) is a penalty objective function. For this reason the method according to the invention will also be referred to as the penalty method.

5 The invention consists of a minimization procedure involving a cost functional comprising of a data-misfit term and a penalty term that measures how accurately the fields satisfy the PDE. The method is composed of two alternating steps, namely the solution of a system of equations forming the discretization of the data-augmented PDE, and the solution of physical model parameters from the PDE itself given the field that solves the data-augmented system and an estimate for the

10 sources.

Compared to the known all-at-once approaches to PDE-constrained optimization, there is no need to update and store the fields for all sources leading to significant memory savings. As in the all-at-once-approach, the proposed method explores a larger search space and is therefore less sensitive to initial estimates for

15 the physical model parameters. Furthermore the method according to the invention solves the data-augmented PDE for the field in step (ii) making the method less prone to a cycle skip resulting in a trap at a local minimum. Contrary to the known reduced formulation, the method according to the invention does not require the solution of an adjoint PDE, effectively halving the number of PDE solves and

20 memory requirement. As in the reduced formulation, fields can be computed independently and aggregated, possibly in parallel.

Reference will be made to Figure 1. The method according to the invention for determining the physical model parameters from measured data comprises the steps (i)-(iii).

25 In step (i) an initial model may be found by methods know to one skilled in the art. as for example velocity analysis and traveltime tomography.

In step (ii) a system of equations is set up for the field, comprising of the discretized PDE, the sampling operator, the source function and the observed data and solve the data-augmented PDE in a suitable manner to obtain a field that both

30 satisfies the PDE and fits the data to some degree. Suitably a trade off parameter λ is used in the process of balancing the data- and PDE-misfit terms. In other words step

(ii) may be performed by minimization of Equation (4) with respect to the fields $\mathbf{u}_i$ by solving for each i the data-augmented PDE as defined in Equation (5) to obtain a field $\overline{\mathbf{u}} = [\overline{\mathbf{u}}_1; \cdots ; \overline{\mathbf{u}}_M]$,

5   (5) $\begin{pmatrix} \lambda A_i(\mathbf{m}) \\ P_i \end{pmatrix} \mathbf{u}_i = \begin{pmatrix} \lambda \mathbf{q}_i \\ \mathbf{d}_i \end{pmatrix}.$

This data-augmented PDE can be interpreted as a regularized version of the original PDE forcing the field to fit the data while solving the PDE. Given these fields, a modified objective is defined, which solely depends on **m.**

In step (iii) a system of equations is set up by using the PDE, the source

10   function and the field obtained in step (ii) and solve this system of equations in a suitable manner to obtain an update of the physical model parameters. The physical model paramaters may be updated subject to prior constraints.

Step (iii) may be performed by calculation of a gradient from a modified objective, defined in Equation (6). Note that the dependency of $\mathbf{u}_i$ on **m** does not

15   appear in the gradient because $\nabla_{\mathbf{u}} \phi_\lambda = 0$ by virtue of having solved Equation (5). We have

(6) $\overline{\phi}_\lambda(\mathbf{m}) = \phi_\lambda(\mathbf{m}, \overline{\mathbf{u}}(\mathbf{m})),$

wherein $\overline{\mathbf{u}}$ is the field obtained in step (ii) and using the expression in Equation (7)

20   (7) $\nabla_{\mathbf{m}} \overline{\phi}_\lambda(\mathbf{m}) = \nabla_{\mathbf{m}} \phi_\lambda(\mathbf{m}, \overline{\mathbf{u}}) = \sum_{i=1}^{M} \lambda^2 G_i(\mathbf{m}, \overline{\mathbf{u}}_i)^* (A_i(\mathbf{m})\overline{\mathbf{u}}_i - \mathbf{q}_i)$

and calculation of a sparse approximation of the Hessian (H) by ignoring the $\mathcal{O}(\lambda^4)$ terms in Equation (8)

(8) $\nabla^2 \overline{\phi}_\lambda(\mathbf{m}) = \sum_{i=1}^{M} \lambda^2 G_i^* G_i - \lambda^4 G_i^* A_i (P_i^T P_i + \lambda^2 A_i^* A_i)^{-1} A_i^* G_i,$

and by summing over all sources, and calculation of an update for the

25   physical model parameters using the calculated gradient and the calculated inversion of the sparse approximation of the Hessian.

If the $\mathcal{O}(\lambda^4)$ terms are neglected, the Hessian

$$H = \sum_{i=1}^{M} \lambda^2 G_i^* G_i$$

becomes sparse and typically diagonal dominant. Given these expressions for the gradient and approximate Hessian, the physical parameter updates become

(9) $\delta\mathbf{m} = -H^{-1}\nabla_{\mathbf{m}}\overline{\phi}_{\lambda}(\mathbf{m})$.

The gradient and Hessian can be formed without storing all the fields by assembling the terms in a running sum. Thus, the fields can be solved independently and in parallel while aggregating the results. Therefore the method is suitably performed wherein an update for the physical model parameters in step (iii) is calculated by solving the data-augmented PDEs of step (ii) in parallel and aggregating the gradient and Hessian of step (iii) across all sources. In such an approach equations (7) and (8) are solved in parallel.

The above basic iterative method minimizes the objective of equation (6) thereby avoiding to have to store all 2M fields and comprises of the following steps:

1. select an appropriate initial model $\mathbf{m}^0$ and trade-off parameter λ,

2. solve the data-augmented PDEs $\begin{pmatrix}\lambda A_i(\mathbf{m}^k) \\ P_i\end{pmatrix}\mathbf{u}_i = \begin{pmatrix}\lambda\mathbf{q}_i \\ \mathbf{d}_i\end{pmatrix}$ for all i,

3. compute the gradient $\mathbf{g} = \sum_{i=1}^{M}\lambda^2 G_i(\mathbf{m}^k, \mathbf{u}_i)^*(A_i(\mathbf{m}^k)\overline{\mathbf{u}}_i - \mathbf{q}_i)$ by aggregrating the results of step 2 over all i,

4. compute the (approximate) Hessian $H = \sum_{i=1}^{M}\lambda^2 G_i^* G_i$ by aggregrating the results of step 2 over all i,

5. compute the update $\delta\mathbf{m} = -H^{-1}\mathbf{g}$,

6. determine a steplength α,

7. update $\mathbf{m}^{k+1} = \mathbf{m}^k + \alpha\delta\mathbf{m}$ and increase the trade-off parameter λ and repeat steps 2-7 until a predetermined stopping criterion is met.

In the method according to the invention the steps (ii) and (iii) are repeated until a predetermined stopping criterion is met. Such a stopping criterion may be obtained, given initial estimates for the physical model parameters and the source function, via a local optimization method that utilizes the misfit value, gradient and Hessian as obtained in steps (ii) en (iii) in the context of a steepest-descent method, or, a Quasi/Gauss/full-Newton method, or a trust-region method or obtained via (bb) a global search method, that utilizes values of the modified objective of

equation (6) in the context of a simplex-based method or a simulated-annealing-based method. In the above method the misfit value, sometimes referred to as the misfit function represents a single value or number which expresses the misfit which is minimized as a function of m and u.

5   Suitably the trade-off parameter λ is increased at a predefined rate ensuring convergence of the algorithm to a solution of the PDE-constrained optimization problem according to equation (1)

$$(1) \quad min_{\mathbf{m},\mathbf{u}} \sum_{i=1}^{M} \frac{1}{2} \parallel P_i\mathbf{u}_i - \mathbf{d}_i \parallel_2^2 \quad \text{s.t.} \quad A_i(\mathbf{m})\mathbf{u}_i = \mathbf{q}_i, \quad i = 1 \cdots M$$

10   Thus the invention is also directed to a computer-implemented method for obtaining a physical model having physical model parameters wherein solutions to one or more partial-differential-equations (PDE's) are calculated, wherein the PDE's are constrained by observed data from a system whose response to a known source function is modeled by solutions of those PDEs for a given physical model using

15   physical model parameters, and these solutions are subsequently used to update the physical model parameters, comprising the following steps:

        (a) discretization of the PDE resulting in the system matrices $A_i(\mathbf{m})$ in Equation (4),

$$(4) \quad \phi_\lambda(\mathbf{m}, \mathbf{u}) = \sum_{i=1}^{M} \frac{1}{2} \parallel P_i\mathbf{u}_i - \mathbf{d}_i \parallel_2^2 + \frac{\lambda^2}{2} \parallel A_i(\mathbf{m})\mathbf{u}_i - \mathbf{q}_i \parallel_2^2$$

20   parameterized by the physical model parameters $\mathbf{m}$,

        wherein $\mathbf{m} \in \mathbb{C}^N$ is a vector of length N with gridded medium parameters,

        $i = 1 \cdots M$ is the experiment index,

        $\mathbf{d}_i \in \mathbb{C}^K$ are the observed data with K the number of samples,

        $A_i(\mathbf{m})$ is the system matrix,

25        $\mathbf{q}_i \in \mathbb{C}^N$ represent the discretized source vectors,

        $\mathbf{u}_i \in \mathbb{C}^N$ are the corresponding discretized fields,

        P_i is the detection operator for the ith source experiment,

        λ is a trade-off parameter

(b) discretization of the source function resulting in the source vector $\mathbf{q}_i$ in Equation (4),

(c) implementation of a linear operator that models the physical properties of the receivers for each source experiment, resulting in P_i in Equation (4),

5   (d) definition of the penalty objective function in Equation (4) consisting of a least-squares data-misfit term, $\| P_i\mathbf{u}_i - \mathbf{d}_i \|_2^2$, and a λ-weighted PDE-residual term, $\| A_i(\mathbf{m})\mathbf{u}_i - \mathbf{q}_i \|_2^2$,

(e) minimization of Equation (4) with respect to the fields $\mathbf{u}_i$ by solving for each i the data-augmented PDE as defined in Equation (5),

10

$$(5) \quad \begin{pmatrix} \lambda A_i(\mathbf{m}) \\ P_i \end{pmatrix} \mathbf{u}_i = \begin{pmatrix} \lambda \mathbf{q}_i \\ \mathbf{d}_i \end{pmatrix}$$

which consists of the system matrix for a given model for the physical parameters, scaled by the trade-off parameter λ, and the data-acquisition operator

15   defined under step c, wherein the right-hand side of this augmented system consists of the source function defined under step b, scaled by the trade-off parameter, and the observed data organized in a vector,

(f) calculation of the gradient from the modified objective, defined in Equation (6),

20     $(6) \quad \overline{\phi}_\lambda(\mathbf{m}) = \phi_\lambda(\mathbf{m}, \overline{\mathbf{u}}(\mathbf{m})),$

using the expression in Equation (7)

$(7) \quad \nabla_{\mathbf{m}}\overline{\phi}_\lambda(\mathbf{m}) = \nabla_{\mathbf{m}}\phi_\lambda(\mathbf{m}, \overline{\mathbf{u}}) = \sum_{i=1}^{M} \lambda^2 G_i\,(\mathbf{m}, \mathbf{u}_i)^*(A_i(\mathbf{m})\overline{\mathbf{u}}_i - \mathbf{q}_i).$

that involves the summation over all sources of the adjoint of the Jacobian with respect to the physical medium properties of the field computed under step e

25   and multiplied by the system matrix, applied to the PDE-residual term defined under step d,

(g) calculation of a sparse approximation of the Hessian by ignoring the $\mathcal{O}(\lambda^4)$ terms in Equation (8)

$(8) \quad \nabla^2\overline{\phi}_\lambda(\mathbf{m}) = \sum_{i=1}^{M} \lambda^2\, G_i^* G_i - \lambda^4 G_i^* A_i(P_i^T P_i + \lambda^2 A_i^* A_i)^{-1} A_i^* G_i,$

and by summing over all sources, and

(h) calculation of an update for the physical model parameters using the gradient calculated under step f and the inversion of the approximate Hessian calculated under step g.

5   A comparison of the constrained, reduced and penalty formulations in terms of the computational complexity for FWI is given in the table below, wherein M represents the number of source experiments and N is the number of discretization points within each field.

	PDE's	Storage	Gauss-Newton update
constrained	0	$M \times N$	solve sparse symmetric, possibly indefinite system in $(M + 1) \times N_g$ unknowns
reduced	$2M$	$2N$	solve matrix-free linear system in N unknowns, requiring M PDE solves per mat-vec
penalty	M	N	solve sparse SPSD system in N unknowns

10   A key step in the penalty method is the solution of the augmented PDE (5). While one can make use of factorization techniques for small-scale applications to efficiently solve the data-augmented PDE for multiple right-hand-sides, industry-scale applications, such as large, sparse, mildly overdetermined systems, will typically require (preconditioned) iterative solution of such systems. Suitably the
15   calculation of solutions of the data-augmented system defined in Equation (5) having multiple right-hand-sides is performed using solution techniques that exploit multiple right-hand-sides. Preferably the solution technique involves solving for the multiple right-hand-sides in parallel, by reusing the QR factors of the data-augmented PDE, or by using block-iterative Krylov methods. More preferably the
20   data-augmented PDE, such as for example the data-augmented wave equation, is solved by direct solvers based on QR factorizations, or by iterative solvers based on

(randomized) (block) Kaczmarz, or by iterative solvers based on the parallel row-projected block CARP-CG method.

Examples of suitable methods for the above is a generic accelerated row-projected method described by Björck, Å., and T. Elfving. 1979. "Accelerated
5   projection methods for computing pseudoinverse solutions of systems of linear equations." *BIT* 19 (2) (jun): 145–163. doi:10.1007/BF01930845, and Gordon, Dan, and Rachel Gordon. 2013. "Robust and highly scalable parallel solution of the Helmholtz equation with large wave numbers." *Journal of Computational and Applied Mathematics* 237 (1) (jan): 182–196. doi:10.1016/j.cam.2012.07.024 which
10   proved successful in seismic applications and can be easily extended to deal with overdetermined systems (Censor, Yair, Paul P. B. Eggermont, and Dan Gordon. 1983. "Strong underrelaxation in Kaczmarz's method for inconsistent systems" *Numerische Mathematik* 41 (1) (feb): 83–92. doi:10.1007/BF01396307) and multiple right-hand-sides by using block-Krylov methods.

15   Time-domain formulation: An application of the penalty method to static PDEs, in which case a complete field $\mathbf{u}_i$ for one source can be stored is straightforward. For a time-varying PDE, the PDE (after spatial discretization) can be written as $M(\mathbf{m})\mathbf{u}'(t) + S\mathbf{u}(t) = \mathbf{q}(t)$, and the system matrix $A(\mathbf{m})$ contains the matrices M and S as blocks. It is no longer feasible to store the fields for all time
20   steps and the matrix is inverted some form of time-stepping. The data-augmented PDE involves an extra equation of the form $P\mathbf{u}(t) = \mathbf{d}(t)$. While one can in principle formulate a large overdetermined system for the wavefield at all timesteps, this is not feasible and a suitable time-stepping strategy will have to be developed to solve the augmented PDE without storing the fields for all time steps. One possible avenue
25   is the use of (implicit) QR factorization to form a block lower triangular matrix that is conducive to solution via time-stepping. Another possibility is to form the Normal equations, leading to a banded system that can be solved efficiently by forward and backward time-stepping. Thus the calculation of solutions of the data-augmented system defined in Equation (5) based on a time-dependent PDE may be performed
30   using a time-stepping algorithm.

The computational cost may be reduced by using recently proposed dimensionality reduction/random-trace-estimation techniques that essentially reduce the number of right-hand-sides of the PDE by random subselection or aggregation as described in WO2011160201, US20100018718 and in Avron, Haim, and Sivan Toledo. "Randomized algorithms for estimating the trace of an implicit symmetric positive semi-definite matrix." Journal *of the ACM (JACM)* 58.2 (2011): 8 and in Haber, Eldad, Matthias Chung, and Felix Herrmann. 2012. "An Effective Method for Parameter Estimation with PDE Constraints with Multiple Right-Hand Sides." SIAM Journal on Optimization 22 (3) (jul): 739–757, doi:10.1137/11081126X. Suitably the number of sources of the source field and/or receivers of the detection operator P_i are reduced. Preferably the number of sources of the source field and/or receivers of the detection operator P_i are reduced by a method comprising a source/receiver-subset selection procedure given by Equation (10)

(10) $\quad \tilde{\mathbf{q}}_i = \sum_{j=1}^{M} w_{ij}\, \mathbf{q}_j, \quad \tilde{\mathbf{d}}_i = \sum_{j=1}^{M} w_{ij}\, \mathbf{d}_i,$

where $i = [1,2,\dots,M']$ ($M' << M$) and w_{ij} are given by

1. $\quad w_{ij} = \delta_{ij}$ for a randomly chosen $j \in [1, M]$, or by

2. $\quad$ random Gaussian weights, or by

3. $\quad$ Rademacher random variables $w_{ij} \in \{-1,1\}$, or by

4. $\quad$ random phases $w_{ij} = exp(\sqrt{-1}a_{ij})$, $a_{ij} \in [-\pi, \pi]$ or by other randomly drawn weights used in sketching techniques, and based on various types of randomized separable, or, nonseparable source/receiver encodings with random signs, Gaussian weights, random phase rotations, or random time shifts, followed by superposition, or various types of randomized separable, or, nonseparable selections of sources/receivers

using uniform random sampling with or without replacement, jitter sampling with or without replacement, or importance sampling with and without replacement.

The subset selection may be controlled by either redrawing the subsets,

5   and/or by increasing the cardinality of the subsets after each gradient calculation in step (iii) as described in Friedlander, Michael P., and Mark Schmidt. 2012. "Hybrid Deterministic-Stochastic Methods for Data Fitting." SIAM Journal on Scientific Computing 34 (3) (may): A1380–A1405. doi:10.1137/110830629.; T. van Leeuwen and Herrmann 2012).

10   The formulation in Equation (4) can if necessary be improved by replacing the Euclidian norms for the misfit functionals by misfit functionals that are robust with respect to outliers in the observed data or measure the misfit in (weighted) matrix norms, for example more general (weighted) two norms, or by robust (weighted) norms such as the one-norm, or by Schatten p matrix norms, such as the

15   Nuclear norm. For matrix norms, the sums over the M individual source experiments in Equation (4) are replaced by matrix norms taken over wavefields organized as matrices. Wavefields for each time-harmonic experiment sharing the same receivers are organized as columns of these matrices.

The computational costs of these improvements may be reduced by using

20   (weighted) random trace-norm estimation techniques for the two-norm, or by using recently proposed and above referred to sketching techniques, extending random-trace estimation to other than two norms as described by Clarkson, K. L., Drineas, P., Magdon-Ismail, M., Mahoney, M. W., Meng, X., & Woodruff, D. P. (2013, January), The Fast Cauchy Transform and Faster Robust Linear Regression, In *SODA* (pp. 466-

25   477), or by sketching techniques for the estimation of matrix norms such as the Schatten norm as described by Yi Li, Hu L. Nguyen, and David P. Woodruff, "On Sketching Matrix Norms and the Top Singular Vector", 2014.

The error induced by the randomized subset selection may be controlled by either redrawing the subsets, and/or by increasing the cardinality of the subsets

30   after each gradient calculation in step (iii).

In step (iii) the physical model parameters may be updated subject to prior constraint. This update is also referred to as regularization in the physical model parameters and can be used to add prior knowledge about the physical model parameters, such as for example minimum or maximum values. One way of achieving this is by adding a suitable regularization term R(m) to equation (4) resulting in equation (11).

(11)

$$min_{\mathbf{m},\mathbf{u}}\phi_\lambda(\mathbf{m},\mathbf{u}) = \sum_{i=1}^{M} \frac{1}{2} \parallel P_i\mathbf{u}_i - \mathbf{d}_i \parallel_2^2 + \frac{\lambda^2}{2} \parallel A_i(\mathbf{m})\mathbf{u}_i - \mathbf{q}_i \parallel_2^2 + R(\mathbf{m}).$$

Regularization by transform-domain sparsity promotion via (weighted) one-norm minimization may be included, or regularization by TV-norm minimization may be included or regularization by Sobolev-norm minimization may be included.

Also, regularization techniques on the (Gauss-Newton) subproblems can be included. This includes for example ℓ_1 regularization as proposed by Li et al. (2012) and ℓ_2 regularization as is used in trust-region methods. It is to be understood that these Euclidean ℓ_2 norms can be replaced by other metrics depending on the function spaces to which $\mathbf{u}$ and $\mathbf{m}$ belong.

Penalties : Penalties other than the ℓ_2 norm on either the data-misfit or the constraint can be included in the formulation (4). However, this will most likely prevent us from solving for the fields efficiently via a system of equations (5). Still, most alternative penalties may be approximated by a weighted ℓ_2 norm, in which case a system like (5) *can* be formed as in (12):

(12) $\begin{pmatrix} \lambda W_1 A_i(\mathbf{m}) \\ W_2 P_i \end{pmatrix} \mathbf{u}_i = \begin{pmatrix} \lambda W_1 \mathbf{q}_i \\ W_2 \mathbf{d}_i \end{pmatrix},$

possibly leading to an iteratively re-weighted least-squares approach.

The method according to the invention may also be used when some aspects of the experiment are not known but can be described by a set of parameters. Such parameters are sometimes referred to as nuisance parameters and they can be estimated in addition to the steps (ii) and (iii). Eexamples of nuisance parameters are the source-weights in seismic applications or the time-signature of the source function. Suitably the source weights are calculated, given the current physical

model parameters, and the solution of the data-augmented PDE as defined in step (ii), by minimizing Equation (13) for each i with respect to the unknown source weight. The penalty objective, in this case becomes

(13) $\phi_\lambda(\mathbf{m}, \mathbf{u}, \theta) = \frac{1}{2} \sum_{i=1}^{M} \| \theta_i P_i \mathbf{u}_i - \mathbf{d}_i \|_2^2 + \lambda^2 \| \theta_i A_i(\mathbf{m}) \mathbf{u}_i - \mathbf{q}_i \|_2^2,$

5   wherein θ_i represents the source scaling nuisance parameter. The field may be solved first from (5) and subsequent minimization over θ for the given fields is trivial as a closed-form solution is available:

$$\theta_i = \frac{\mathbf{u}_i^*(P_i^* \mathbf{d}_i + \lambda^2 A_i^* \mathbf{q}_i)}{\| P_i \mathbf{u}_i \|_2^2 + \lambda^2 \| A_i \mathbf{u}_i \|_2^2}.$$

This approach can be generalized to more complicated situations in which a

10   closed-form solution is not available as described by Aravkin, A. Y., and T. van Leeuwen. 2012. "Estimating nuisance parameters in inverse problems." *Inverse Problems* 28 (11): 115016.

Suitably the method makes use of so-called Uncertainty Quantification, which provides information on the uncertainties, via probability density functions or

15   attributes thereof such as variances, for the physical model at each grid point. Uncertainty quantification is typically based on a Gaussian model for the probability-density function over the model-space given by

(14) $\pi(\mathbf{m}) \propto exp(-(\mathbf{m} - \mathbf{m}^*)H^{-1}(\mathbf{m} - \mathbf{m}^*)),$

where $\mathbf{m}^*$ is a minimizer of the penalty objective and H is the (Gauss-

20   Newton) Hessian of the penalty objective function. In this case, the Hessian can be easily approximated by a sparse matrix (see Equation (8)) and it's inverse can be computed via factorization techniques. This allows for extraction of various statistics of $\pi(\mathbf{m})$ as well as generation of random models according to $\pi(\mathbf{m})$

The method may find suitable use in the field of PDE constrained

25   optimization problems such as in process control, medical imaging, non-destructive testing, radar imaging, remote sensing, radiative transfer and design. More preferably the method is used in the field of travel-time tomography in geophysical prospecting, in the field of electromagnetic inversion in geophysical prospecting, in the field of inversion of gravity data in geophysical prospecting and in the field of

wave-equation based inversion in geophysical prospecting and wherein the physical model is a model of a geological area. The model may be used by geologists, reservoir engineers or drilling engineers to help them understand the geological area and the relevant hydrocarbon reservoir.

5   In an even more preferred use the method is used in the field of wave-equation based inversion in geophysical prospecting and wherein the model of a geological area has poro/visco-elastic model parameters. Wave-equation based inversion methods include:

   - Wave-equation based migration, which is the preferred method for imaging

10 reflected waves. This can be achieved by applying steps (ii) and (iii) of the method according to the invention to suitably processed data and a suitable initial model of the visco/poro-elastic parameters.

   - Linearized amplitude-versus-offset/angle/ray-parameter inversion, which is the preferred method for reservoir characterization. This can be achieved by

15 applying steps (ii) according the invention and using the field obtained in step (ii) and the corresponding PDE-residual to form image gathers as a function of offset/angle/ray-parameter and fitting the amplitude behavior to linearized reflection coefficients.

   - Wave-equation based migration velocity analysis, which is the preferred

20 method for obtaining a smooth model of the visco/poro-elastic parameters for use as an initial model for FWI. This can be achieved by applying step (ii) according to the invention and a modification of step (iii) according to the invention in which the field obtained in step (ii) is correlated with the PDE-residual at non-zero lags/offsets to form image gathers. Having contracted these image gathers, an

25 update of the visco/poro-elastic parameters can be extracted using techniques known to those trained in the art of velocity analysis.

   - Full waveform inversion, which is the preferred method for obtained high-resolution models of the visco/poro-elastic parameters in geologically complex areas. This can be achieved by iteratively applying steps (ii) and (iii) according to

30 the invention on suitably preprocsessed data and possibly including various manners of continuation in frequency/offset/depth.

The differences between the current algorithms for full waveform inversion and the method according to the invention is illustrated in Figures 2 and 3. Figure 2 illustrates the known waveform inversion approach for a computer implemented method for geophysical prospecting. The methods is aimed at obtaining a physical

5 model (1) having physical model parameters wherein solutions to one or more partial-differential-equations (PDE's) are calculated, wherein the PDE's are constrained by observed data (2) from a system whose response to a known source function (3) is modeled by solutions of those PDEs for a given physical model using physical model parameters. In this method one may start from an appropriate initial

10 model (4). Subsequently the wave propagation is simulated (5) using the source function (3) and the model (1), for example by means of the finite differences methodology. Subsequently predicted data (6) may be calculated using the simulated wave-propagation of step (5). In step (7) the model (1) is updated using the difference between the observed data (2) and the predicted data (6). The steps

15 of simulating the wave propagation and updating the model are repeated until a predetermined stopping criterion is met.

Figure 3 illustrates the method according to the present invention. As in Figure 1 it shows a computer-implemented method for obtaining a physical model (10) having physical model parameters wherein solutions to one or more partial-

20 differential-equations (PDE's) are calculated, wherein the PDE's are constrained by observed data (2) from a system whose response to a known source function (3) is modeled by solutions of those PDEs for a given physical model using physical model parameters. In a step (i) an appropriate initial model (10) is selected. In a step (ii) data-augmented wave-equation (11) is formulated using the source function (3) and

25 wherein the solution is constrained to fit the observed data (2) to obtain reconstructed wavefields, also referred to as field (12). In a step (iii) a wave-equation residual (13) is computed using the source function (3) and the field (12) and use the wave-equation residual (13) to update the physical model (10). Steps (ii)-(iii) are repeated until a predetermined stopping criterion is met.

30 Figure 3 shows an approach for full waveform inversion which includes the wave-equation as an additive regularization term. Applicants found that this

regularization term controls the trade-off between data-fit and accuracy of the solution of the wave-equation. The resulting optimization problem can be solved efficiently with this approach. Furthermore this approach avoids having to solve an adjoint wave-equation and the approach avoids solving the wave-equation exactly

5   and thus leads to a less non-linear problem.

In such a seismic application, given an initial model for the physical parameters, and an estimate for the source function, a basic implementation of the penalty method as described above for seismic applications may involve the following steps:

10   1.   Solve the data-augmented wave equation (5) for all sources and compute the PDE residuals given by $(A_i(\mathbf{m})\overline{\mathbf{u}}_i - \mathbf{q}_i)$.

2.   Correlate the wavefield $\overline{\mathbf{u}}_i$ with the PDE residual according to Equation (7), and apply the zero-time imaging condition ,by summing over the frequencies in the time-harmonic formulation, and aggregate over the sources to

15   calculate the gradient.

3.   Correlate the wavefield $\overline{\mathbf{u}}_i$ with itself according to Equation (8), and apply the zero-time imaging condition, and aggregate over the sources to calculate the (approximate) Hessian.

4.   Apply a conditioning, for example scaling, smoothing or inverse

20   Hessian, to the gradient to obtain the model update and update the model.

The above procedure is repeated for the updated model parameters until a predetermined stopping criterion is met, suitably wherein the data-misfit functional is decreased sufficiently or until the model updates become sufficiently small. The above formulation is conducive to be solved by commonly used optimization

25   methods including gradient descent, nonlinear conjugate gradients, l-BFGS, and Gauss-Newton. The costs of these methods are proportional to the number of iterations times the number of source experiments, which determine the number of PDE solves. The above formulation is also conducive to dimensionality reduction techniques aimed at reducing the number of PDE solves.

30   As demonstrated in the examples below, the trade-off parameter λ controls the width of the basin of attraction of the penalty objective function. By using a

continuation method where the trade-off parameter is increased from a suitable starting value, the solution of the penalty method converges to the solution of the constrained method. For example, a suitable starting value for the trade-off parameter can be found by checking for cycle skips in the data residual.

5   The procedure described above can be used in conjunction with conventional FWI workflows, including:

1.   multi-scale inversion, where the algorithm is applied to bandpass filtered data sweeping from low to high frequencies.

2.   Laplace-domain damping, where the algorithm is applied to time-

10   damped data, sweeping from small to larger time windows, and

3.   offset-continuation, where the offset range of the data is gradually increased.

The above procedure is applicable to any discretization of a wave equation that models elastic waves in media that are viscous and may contain pores filled

15   with a mixture of fluids and gases.

In view of the above the method when used in the field of wave-equation based inversion in geophysical prospecting may for example be performed as below. The method will use an initial estimate of the poro/visco-elastic model parameters. The method further comprises:

20   -   (aaa) a procedure to determine a suitable value of the trade-off parameter λ such that the initial estimate of the poro/visco-elastic model parameters is within the basin of attraction of the penalty objective function,

-    (bbb) solution of the data-augmented wave equation (5) for all sources and computation of the PDE residuals as in step (ii) and part of step (iii) and wherein

25   the remainder of step (iii) is performed in (ccc) and (ddd):

-    (ccc) computation of the gradient by

 (c1) correlation of the wavefield obtained in (bbb) with the PDE residuals obtained in (bbb),

 (c2) application of the zero-time lag imaging condition,

30   (c3) aggregation over the sources to calculate the gradient,

-    (ddd) computation of an update of the poro/visco-elastic model parameters by

(d1) the gradient of poro/visco-elastic model parameters, scaled by the steplength, or by,

(d2) the gradient of poro/visco-elastic model parameters, scaled by the steplength and the inverse of the approximate aggregated Hessian, or by,

5   (d3) using an l-BFGS approximation of the inverse of the Hessian.

-   (eee) a continuation procedure to gradually increase the trade-off parameter λ.

Preferably the data-augmented wave equation in the above step (bbb) is solved by direct solvers based on QR factorizations, or by iterative solvers based on (randomized) (block) Kaczmarz, or by iterative solvers, for example based on the

10   parallel row-projected block CARP-CG method.

Suitable a continuation method may be used to improve the convergence of the method according the invention. Suitable continuation methods are continuation methods are used that

-   update the coarse scales of the poro/visco-elastic model parameters first

15   by starting at the long wavelengths and using the updated coarse-scale poro/visco-elastic model parameters as warm starts to calculate updates of the poro/visco-elastic model parameters at the finer scales, and/or,

-   update the shallow parts of the poro/visco-elastic model parameters first by starting with data from short time windows after the first arrival and

20   using the updated shallow poro/visco-elastic model parameters as warm starts to calculate deeper updates of the poro/visco-elastic model parameters, and/or,

-   update the acoustic model parameters first by starting with data from narrow offset windows and using the updated acoustic model parameters

25   as warm starts to calculate updates of the elastic model parameters.

Suitably the poro/visco-elastic model parameter updates in step (iii) are conditioned by scaling to compensate for spherical spreading and other amplitude effects, and by linear (anisotropic) smoothing, or by nonlinear anisotropic smoothing by one-norm constraints on the transform domain (curvelet/wavelet)

30   coefficients, or by nonlinear anistropic smoothing by total-variation norm constraints on the updates, or by nonlinear smoothing by anistropic-diffusion.

In one embodiment, the alternating penalty optimization method can suitably be used to conduct reverse-time migration based on the wave-equation and involves the computation of the following gradient:

$$\nabla_{\mathbf{m}}\phi_\lambda(\mathbf{m}_0, \mathbf{u}) = \sum_{i=1}^{M} G_i\left(\mathbf{m}, \mathbf{u}_i\right)^*(A_i(\mathbf{m}_0)\mathbf{u}_i - \mathbf{q}_i) = \sum_{i=1}^{M} J_i^* \, \delta\mathbf{u}_i,$$

5   which involves the action of the adjoint of the Jacobian

(15) $J_i(\mathbf{m}_0, \mathbf{u}_i) = G_i(\mathbf{m}, \mathbf{u}_i)$

with $\mathbf{m}_0$ the simple background model, on the PDE residuals $\delta\mathbf{u}_i = (A_i(\mathbf{m})\mathbf{u}_i - \mathbf{q}_i)$, $i = 1 \cdots M$. As for the reduced formulation, migrated images are constructed by aggregating gradients over all M sources possibly in parallel.

10   However, in the penalty formulation according to the present invention

- there is no need to solve the adjoint system, which effectively halves the memory imprint and required number of wave-equation solves.

- the Jacobian is a sparse matrix, which makes its evaluation computationally efficient compared to the Jacobian of the reduced formulation,

15   which is a dense matrix whose application requires additional wave-equation solves.

In geologically complicated areas hampered by illumination problems, true-amplitude wave-equation least-squares migration is often the imaging method of choice. Least-squares migration involves the solution of the following optimization

20   problem:

$$\min_{\delta\mathbf{m}} \sum_{i=1}^{M} \frac{1}{2} \parallel \mathbf{u}_i - J_i\delta\mathbf{m} \parallel_2^2,$$

which corresponds to solving the normal equations. Because the Jacobian is sparse, so is the Gauss-Newton Hessian, making it cheap to evaluate.

The method when used in the field of wave-equation based inversion in

25   geophysical as described above may also be used by performing a linearized seismic inversion wherein step (ii) and (iii) of the method according to the invention may suitably be performed by

- a reverse-time migration by computing the gradient for a simple model of the poro/visco-elastic parameters, which is given by the action of the adjoint of the Jacobian, defined in Equation (15), on the PDE residual

    $\delta\mathbf{u}_i = (A_i(\mathbf{m})\mathbf{u}_i - \mathbf{q}_i)$, $i = 1\cdots M$, or

5 - a least-squares reverse-time migration by computing the least-squares pseudo-inverse of the Jacobian defined in Equation (15) for a simple model of the poro/visco-elastic parameters and the PDE residual defined under a, or,

- a single iteration of the above described method according to the present invention.

10   Suitably wave-equation-based migration-velocity analysis is conducted and/or a linearized amplitude-versus-offset/angle/ray-parameter inversion is conducted. The method comprises formation of image-gathers from the wavefields that solve the data-augmented wave equation (field) and the PDE residuals that are minimized in order to find an update for the model parameters, used for

15   - quality control of the simple model of the elastic velocity parameters, or,

- compution of velocity parameter updates as part of a migration-velocity analysis procedure, or,

- amplitude-versus-offset/angle/ray-parameter attribute analysis, including two-term amplitude-versus-offset attributes.

20

Examples

The invention will be illustrated by the following non-limiting examples.

These examples are based on a simple 5-point discretization of the 2D Helmholtz operator for frequency ω_i and squared-slowness $\mathbf{m}$

25      $$A_i(\mathbf{m}, \omega_i) := \omega_i^2 \mathrm{diag}(\mathbf{m}) + L,$$

with L the discretized Laplacian. This simplifies the expression for the gradient (7) to

$$\nabla_{\mathbf{m}}\overline{\phi}_\lambda(\mathbf{m}, \mathbf{u}) = \lambda^2 \sum_{i=1}^{M} \omega_i^2 \,\mathrm{diag}(\mathbf{u}_i)^* \delta\mathbf{u}_i$$

and the Hessian (8) can be approximated by

$$H = (\lambda^2) \sum_{i=1}^{M} \omega_i^4 \, \text{diag}(\mathbf{u}_i)^* \text{diag}(\mathbf{u}_i).$$

Because the Hessian is a diagonal matrix, Gaussian-Newton methods for FWI as well as least-squares migration can be implemented straightforwardly.

Example 1

For the first example, a square perturbation embedded in constant velocity background is considered, see Figure 4. Sources and receivers are placed in a cross-well configuration. The corresponding scattered wavefield (i.e., the difference between the wavefield for the perturbed medium and the background medium) at 10 Hz for source at 10,500 is shown in figure 5.

The scattered wavefield is obtained by performing step (ii) of the method of the invention for a constant background and receivers along $z = 10$ is shown in figure 6. The corresponding estimate for **m** as obtained by performing step (iii) of the method according the invention is show in figure 7. Figure 7 shows an image of the estimated model parameters after one iteration, wherein the solution of the augmented wave equation contain "reflected/turned" wavefield components that are reminiscent of wavefield components arising from the solution of the adjoint wave equation.

By including the data-constraint in the PDE some of the structure of the original wavefield is retrieved. This information is subsequently used to derive a new estimate of the model.

Example 2

The penalty method can also be used for imaging purposes. Just as the gradient of the reduced objective yields an image, so does the gradient of the penalty objective. However, for the latter one does not need to solve for an adjoint wavefield. The velocity perturbation shown in figure 8 is considered and data are generated for 101 equispaced sources and receivers located at the top of the model and frequencies $1,2,\ldots,10Hz$. The reverse-time migration according to the prior art

method of Figure 2 is shown in figure 9. The image obtained by using the method according to the invention as illustrated in Figure 3 is shown in figure 10.

Example 3

5   For the next example, a linearly increasing velocity $v_0 + \alpha z$ is considered and the objective functions corresponding to the equation (3) of the prior art and the penalty approaches according to equation (4) according to the present invention as a function of v_0 for various values of λ is plotted in Figure 11.

Figure 11 shows that when the prior art method is used local minima appear
10   in the objective function while when using the method according to the invention and when choosing a favorable λ no local minima are present in the objective function. This shows that the method is less likely to stall.

Relaxing the PDE-constraint by using a small value of λ does help alleviate some of the problems with local minima.

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Example 4

In this example, data for a single source and single frequency is inverted for a 1D velocity profile. The true velocity profile (dotted line in Figure 12) is given by $v(z) = v_0 + \alpha z + \delta v exp(-\beta^2 (z - z_0)^2)$ for values $v_0 = 2000$ m/s, $\alpha = 0.7$ 1/s, $\delta v =$
20   200 m/s, $z_0 = 2000$ m and $\beta = 10^{-3}$. A maximum offset of 3000 m and a frequency of 5 Hz are used. The initial model is a linear gradient with $v_0 = 2000$ m/s and $\alpha = 0.7$ 1/s. For the inversion a simple steepest-descent method with a fixed steplength is used. The result after 1000 iterations is shown in figures 12 and 13. The resulting data are shown in figure 14. Figure 14 shows that the observed data and the fitted
25   data obtained by the method according to the invention overlay, while the data obtained by the reduced method deviate and show evidence of a cycle skip and near receiver index 200. The results indicate that the reduced approach according to the prior art is stuck in a local minimum whereas the penalty approach according to the method according to the invention gives a nice reconstruction. The above results for
30   the method according to the invention may be further improved by using a more

efficient optimization method as described above in this application to speed up the convergence.

CLAIMS

1. A computer-implemented method for obtaining a physical model having physical model parameters wherein solutions to one or more partial-differential-equations (PDE's) are calculated, wherein the PDE's are constrained by observed data from a system whose response to a known source function and known sampling operator is modeled by solutions of those PDEs for a given physical model using physical model parameters, wherein (i) an appropriate initial model is selected, (ii) setup a system of equations referred to as the data-augmented PDE for the field, comprising of the discretized PDE, the sampling operator, the source function and the observed data, and solve the data-augmented PDE in a suitable manner to obtain a field that both satisfies the PDE and fits the data to some degree, (iii) setup a system of equations by using the PDE, the source function and the field obtained in step (ii) and solve this system of equations in a suitable manner to obtain an update of the physical model parameters and repeat steps (ii)-(iii) until a predetermined stopping criterion is met.

2. A method according to claim 1, wherein step (ii) is performed by minimization of Equation (4) with respect to the fields $\mathbf{u}_i$ by solving for each i the data-augmented PDE as defined in Equation (5),

$$(5) \quad \begin{pmatrix} \lambda A_i(\mathbf{m}) \\ P_i \end{pmatrix} \mathbf{u}_i = \begin{pmatrix} \lambda \mathbf{q}_i \\ \mathbf{d}_i \end{pmatrix}$$

and wherein equation (4) is:

$$(4) \quad \phi_\lambda(\mathbf{m}, \mathbf{u}) = \sum_{i=1}^{M} \frac{1}{2} \parallel P_i \mathbf{u}_i - \mathbf{d}_i \parallel_2^2 + \frac{\lambda^2}{2} \parallel A_i(\mathbf{m}) \mathbf{u}_i - \mathbf{q}_i \parallel_2^2$$

parameterized by the physical model parameters $\mathbf{m}$,

wherein $\mathbf{m} \in \mathbb{C}^N$ is a vector of length N with gridded medium parameters,

$i = 1 \cdots M$ is the experiment index with M the number of experiments,

$\mathbf{d}_i \in \mathbb{C}^K$ are the observed data with K the number of samples,

$A_i(\mathbf{m})$ is the system matrix,

$\mathbf{q}_i \in \mathbb{C}^N$ represent the discretized source vectors obtained by discretization of the source function,

$\mathbf{u}_i \in \mathbb{C}^N$ are the corresponding discretized fields,

P_i is the sampling operator for a ith source experiment,

λ is a trade-off parameter

and wherein the least-squares data-misfit term, $\| P_i \mathbf{u}_i - \mathbf{d}_i \|_2^2$, and the λ-weighted PDE-residual term, $\| A_i(\mathbf{m})\mathbf{u}_i - \mathbf{q}_i \|_2^2$, in equation (4) is a penalty objective function to obtain a field $\overline{\mathbf{u}} = [\overline{\mathbf{u}}_1; \cdots ; \overline{\mathbf{u}}_M]$.

3. A method according to claim 2, wherein step (iii) is performed by calculation of a gradient from a modified objective, defined in Equation (6),

(6) $\quad \overline{\phi}_\lambda(\mathbf{m}) = \phi_\lambda(\mathbf{m}, \overline{\mathbf{u}}(\mathbf{m}))$,

wherein $\overline{\mathbf{u}}$ is the field obtained in step (ii) and using the expression in Equation (7)

(7) $\quad \nabla_{\mathbf{m}}\overline{\phi}_\lambda(\mathbf{m}) = \nabla_{\mathbf{m}}\phi_\lambda(\mathbf{m}, \overline{\mathbf{u}}) = \sum_{i=1}^{M} \lambda^2 G_i (\mathbf{m}, \overline{\mathbf{u}}_i)^* (A_i(\mathbf{m})\overline{\mathbf{u}}_i - \mathbf{q}_i)$.

and calculation of a sparse approximation of the Hessian (H) by ignoring the $\mathcal{O}(\lambda^4)$ terms in Equation (8)

(8) $\quad \nabla^2 \overline{\phi}_\lambda(\mathbf{m}) = \sum_{i=1}^{M} \lambda^2 \, G_i^* G_i - \lambda^4 G_i^* A_i (P_i^T P_i + \lambda^2 A_i^* A_i)^{-1} A_i^* G_i$,

and by summing over all sources, and

calculation of an update for the physical model parameters using the calculated gradient and the calculated inversion of the sparse approximation of the Hessian.

4. A method according to any one of claims 2-3, wherein the trade-off parameter λ is increased at a predefined rate ensuring convergence of the algorithm to a solution of the PDE-constrained optimization problem according to equation (1):

$$min_{\mathbf{m},\mathbf{u}} \sum_{i=1}^{M} \frac{1}{2} \parallel P_i \mathbf{u}_i - \mathbf{d}_i \parallel_2^2 \quad \text{s.t.} \quad A_i(\mathbf{m})\mathbf{u}_i = \mathbf{q}_i, \quad i = 1 \cdots M.$$

.

5. A method according to claims 2-4, wherein calculation of solutions of the
    data-augmented system defined in Equation (5) based on a time-dependent
    PDE is performed using a time-stepping algorithm.

6. A method according to any one of claims 1-5, wherein the update for the
    physical model parameters in step (iii) is calculated by solving the data-
    augmented PDEs of step (ii) in parallel and aggregating the gradient and
    Hessian of step (iii) across all sources.

7. A method according to any one of claims 1-6, wherein the number of sources
    of the source field and/or receivers of the detection operator P_i are reduced.

8. A method according to claim 7, wherein the method of reducing the sources
    comprises a source/receiver-subset selection procedure given by Equation
    (10)

    $$(10)....\tilde{\mathbf{q}}_i = \sum_{j=1}^{M} w_{ij} \mathbf{q}_j, \quad \tilde{\mathbf{d}}_i = \sum_{j=1}^{M} w_{ij} \mathbf{d}_i,$$

    where $i = [1,2,\dots,M']$ ($M' << M$) and w_{ij} are given by
    $w_{ij} = \delta_{ij}$ for a randomly chosen $j \in [1, M]$, or by
    random Gaussian weights, or by
    Rademacher random variables $w_{ij} \in \{-1,1\}$, or by
    random phases $w_{ij} = exp(\sqrt{-1}a_{ij})$, $a_{ij} \in [-\pi, \pi]$, or by other randomly drawn
    weights used in sketching techniques,
    and based on
    various types of randomized separable, or,
    nonseparable source/receiver encodings

with random signs, Gaussian weights, random phase rotations, or random time

shifts, followed by superposition, or

various types of randomized separable, or,

nonseparable selections of sources/receivers

5   using uniform random sampling with or without replacement, jitter sampling

with or without replacement, or importance sampling with and without

replacement.

9.   A method according to 8, wherein the effects of the subset selection are

10   controlled by either redrawing the subsets, and/or by increasing the

cardinality of the subsets after each gradient calculation in step (iii).

10.   A method according to any one of claims 1-9, wherein a suitable

regularization term on the physical model parameters is included as in

15   Equation (11):

$$(11)\ min_{\mathbf{m},\mathbf{u}}\phi_\lambda(\mathbf{m},\mathbf{u}) = \sum_{i=1}^{M} \frac{1}{2} \parallel P_i\mathbf{u}_i - \mathbf{d}_i \parallel_2^2 + \frac{\lambda^2}{2} \parallel A_i(\mathbf{m})\mathbf{u}_i - \mathbf{q}_i \parallel_2^2 + R(\mathbf{m}).$$

11.   A method according to claim 10, wherein regularization by transform-

domain sparsity promotion via (weighted) one-norm minimization is

20   included, or wherein regularization by TV-norm minimization is included or

wherein regularization by Sobolev-norm minimization is included.

12.   A method according to any one of claims 2-11, wherein the (weighted) least-

squares misfit terms in Equation (4) are replaced by misfit functionals that

25   are robust with respect to outliers in the observed data or measure the misfit

in (weighted) matrix norms.

13.   A method according to any one of claims 1-12, wherein nuisance parameters

required to compute updates of the physical model parameters are

30   calculated while performing steps (ii) and (iii).

14.   A method according to any one of claims 1-13, wherein the penalty formulation of Equation (4) is solved including uncertainty quantification, comprising generation of random realizations for the physical model parameters from a probability distribution function (14))

$$(14) \quad \pi(\mathbf{m}) \propto exp(-(\mathbf{m} - \mathbf{m}^*)H^{-1}(\mathbf{m} - \mathbf{m}^*)),$$

where $\mathbf{m}^*$ is a minimizer of the penalty objective and H is the (Gauss-Newton) Hessian of the penalty objective function.

15.   A method according to any one of claims 1-14 for use in the field of PDE constrained optimization problems in process control, medical imaging, non-destructive testing, radar imaging, remote sensing, radiative transfer, and design.

16.   A method according to any one of claims 1-14 for use in the field of travel-time tomography in geophysical prospecting, in the field of electromagnetic inversion in geophysical prospecting, in the field of inversion of gravity data in geophysical prospecting and in the field of wave-equation based inversion in geophysical prospecting and wherein the physical model is a model of a geological area.

17.   A method according to claim 16, wherein the use is in the field of wave-equation based inversion in geophysical prospecting and wherein the model of a geological area has poro/visco-elastic model parameters.

18.   A method according to claim 17, wherein a wave-equation-based migration-is conducted.

19.   A method according to claim 17, wherein a linearized amplitude-versus-offset/angle/ray-parameter inversion is conducted.

20. A method according to claim 17, wherein a wave-equation based migration velocity analysis is conducted.

21. A method according to claim 17, wherein a full-wave inversion is conducted.

5

ABSTRACT

The invention is directed to a computer-implemented method for obtaining a physical model having physical model parameters wherein solutions to one or more partial-differential-equations (PDE's) are calculated and wherein (i) an appropriate initial model is selected, (ii) setup a system of equations referred to as the data-augmented PDE for the field, comprising of the discretized PDE, the sampling operator, the source function and the observed data, and solve the data-augmented PDE in a suitable manner to obtain a field that both satisfies the PDE and fits the data to some degree, (iii) setup a system of equations by using the PDE, the source function and the field obtained in step (ii) and solve this system of equations in a suitable manner to obtain an update of the physical model parameters and repeat steps (ii)-(iii) until a predetermined stopping criterion is met.
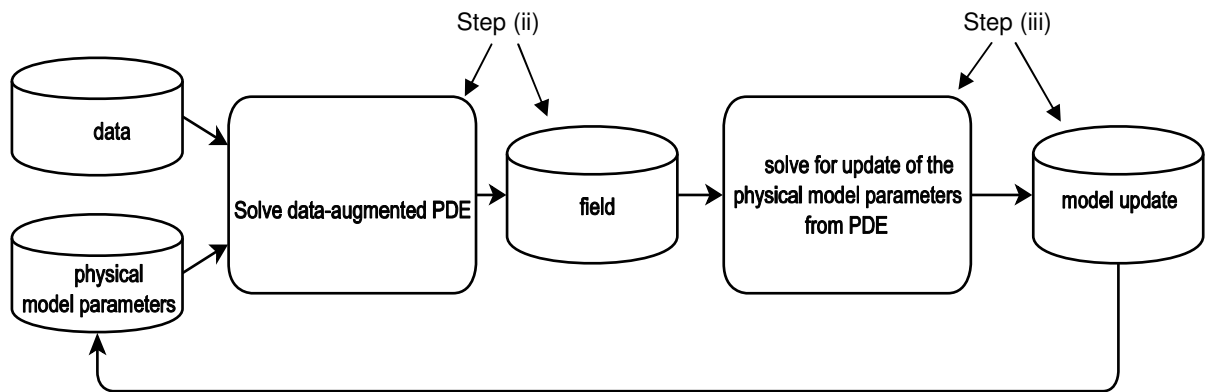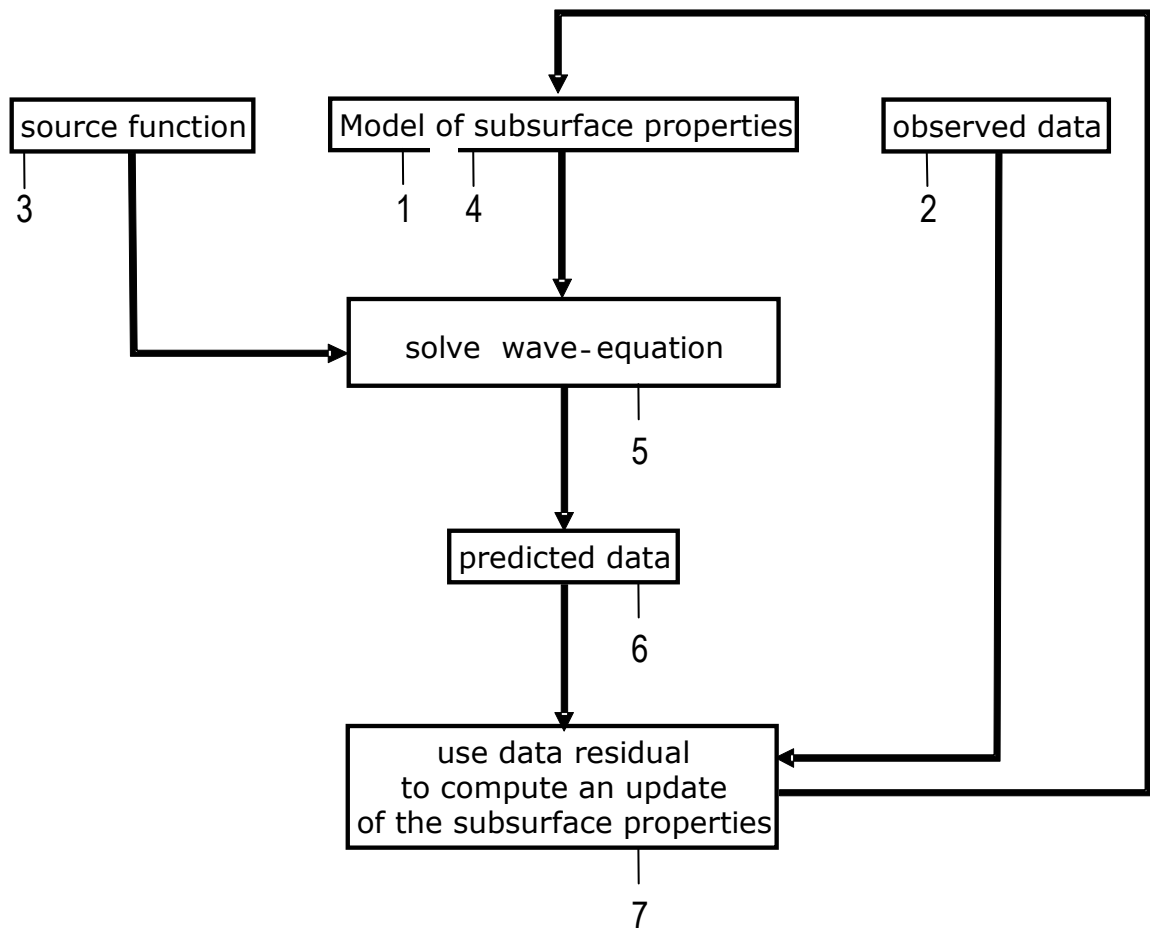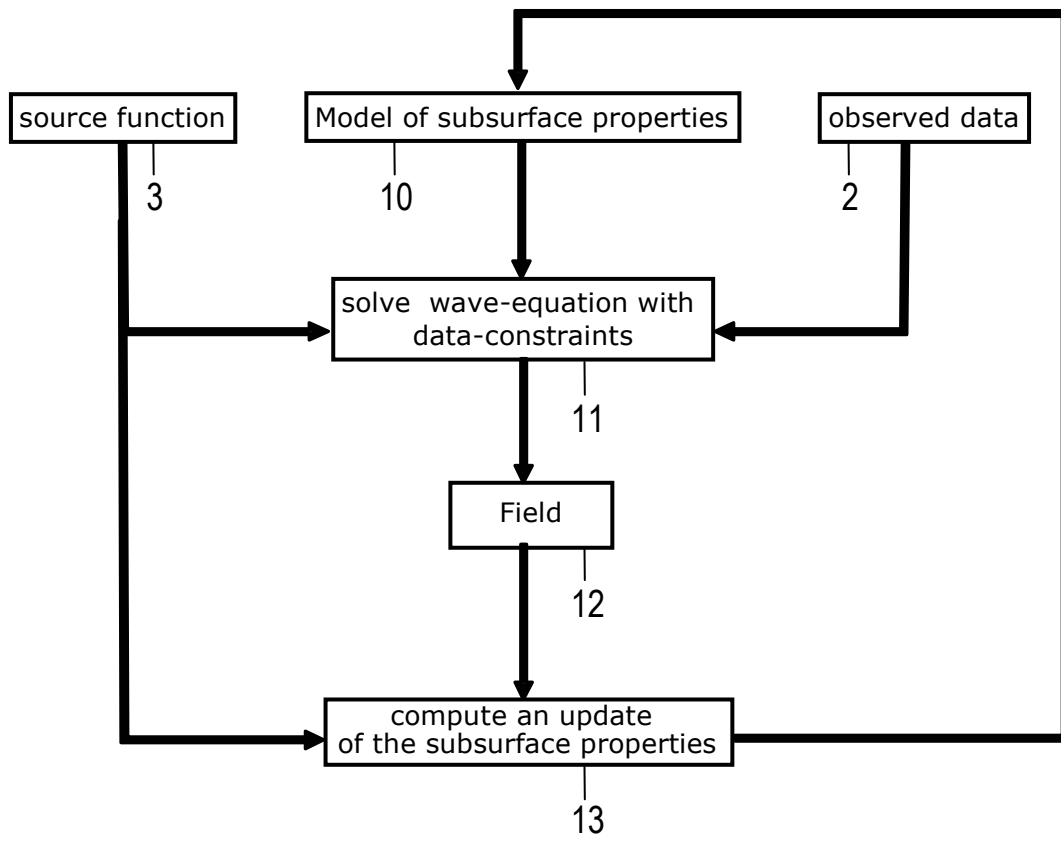
[figure 1 by abstract]

Step (ii)   Step (iii)

```
┌──────────┐
│   data   │
└──────────┘
              ┌──────────────────┐        ┌──────────┐        ┌──────────────────────┐        ┌──────────────┐
              │                  │        │          │        │                      │        │              │
              │ Solve data-      │──────▶ │  field   │──────▶ │ solve for update of  │──────▶ │ model update │
              │ augmented PDE    │        │          │        │ the physical model   │        │              │
┌──────────┐  │                  │        └──────────┘        │ parameters from PDE  │        └──────────────┘
│ physical │  └──────────────────┘                            └──────────────────────┘
│  model   │
│parameters│
└──────────┘
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Fig.1

```
                                  ┌──────────────────────────────────────────────────────┐
                                  │                                                      │
                                  ▼                                                      │
┌──────────────────┐    ┌──────────────────────────────┐    ┌──────────────────┐        │
│  source function │    │ Model of subsurface properties │    │  observed data   │        │
└──────────────────┘    └──────────────────────────────┘    └──────────────────┘        │
         │                      │      │                              │                   │
         3                      1      4                              2                   │
         │                             │                              │                   │
         │                             ▼                              │                   │
         │              ┌──────────────────────────────┐             │                   │
         └────────────▶ │      solve  wave-equation      │             │                   │
                        └──────────────────────────────┘             │                   │
                                       │                             │                   │
                                       5                             │                   │
                                       ▼                             │                   │
                              ┌──────────────────┐                   │                   │
                              │  predicted data  │                   │                   │
                              └──────────────────┘                   │                   │
                                       │                             │                   │
                                       6                             │                   │
                                       ▼                             ▼                   │
                        ┌──────────────────────────────┐                                │
                        │       use data residual       │◀───────────────────────────────┘
                        │    to compute an update       │
                        │  of the subsurface properties  │
                        └──────────────────────────────┘
                                       │
                                       7
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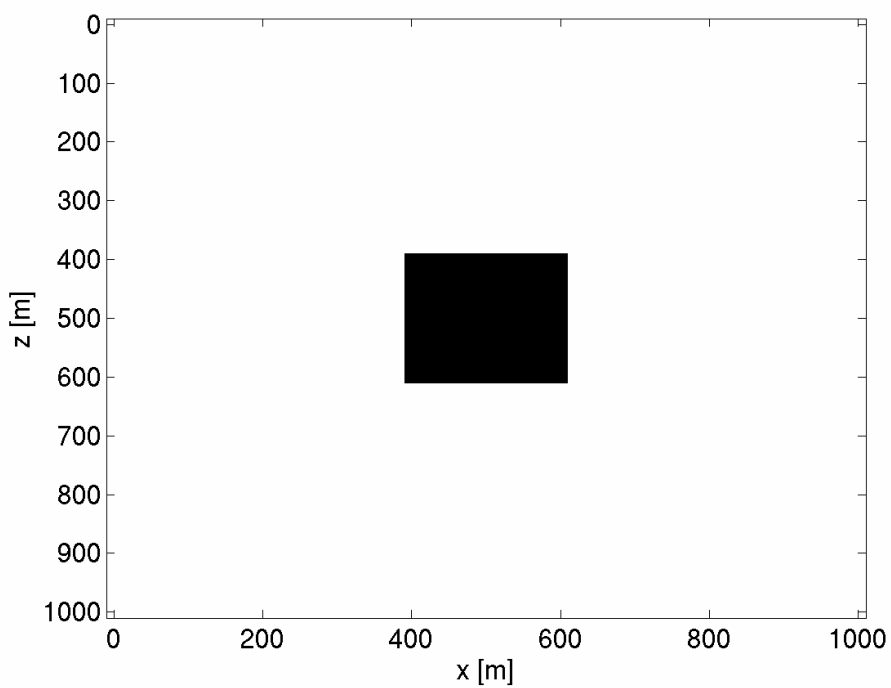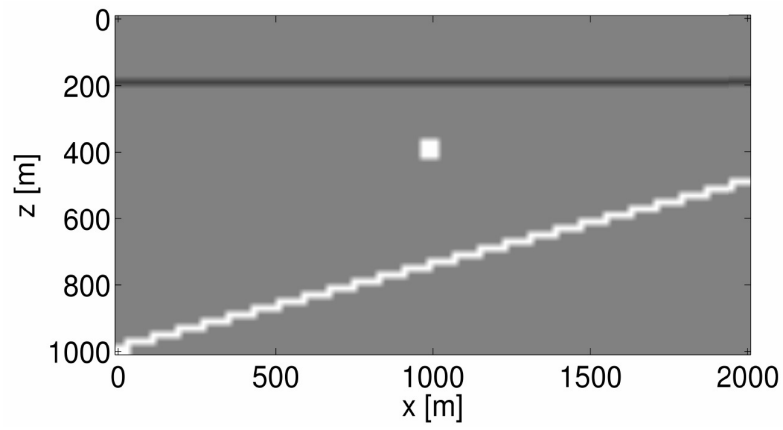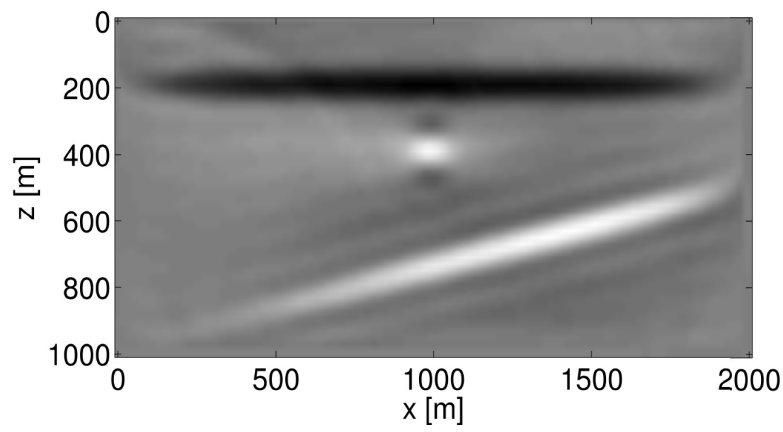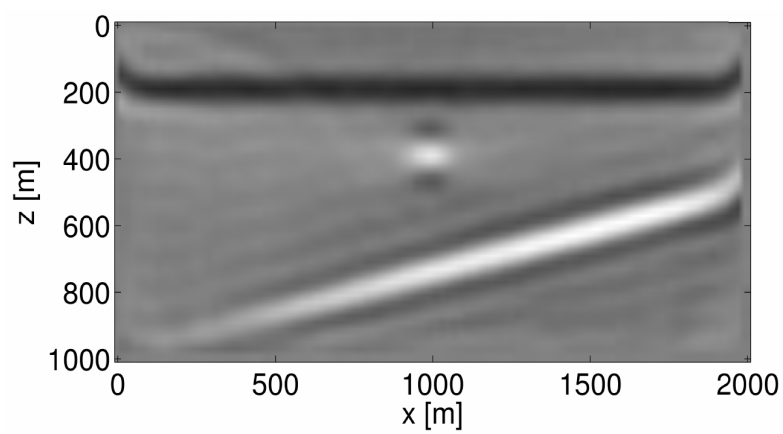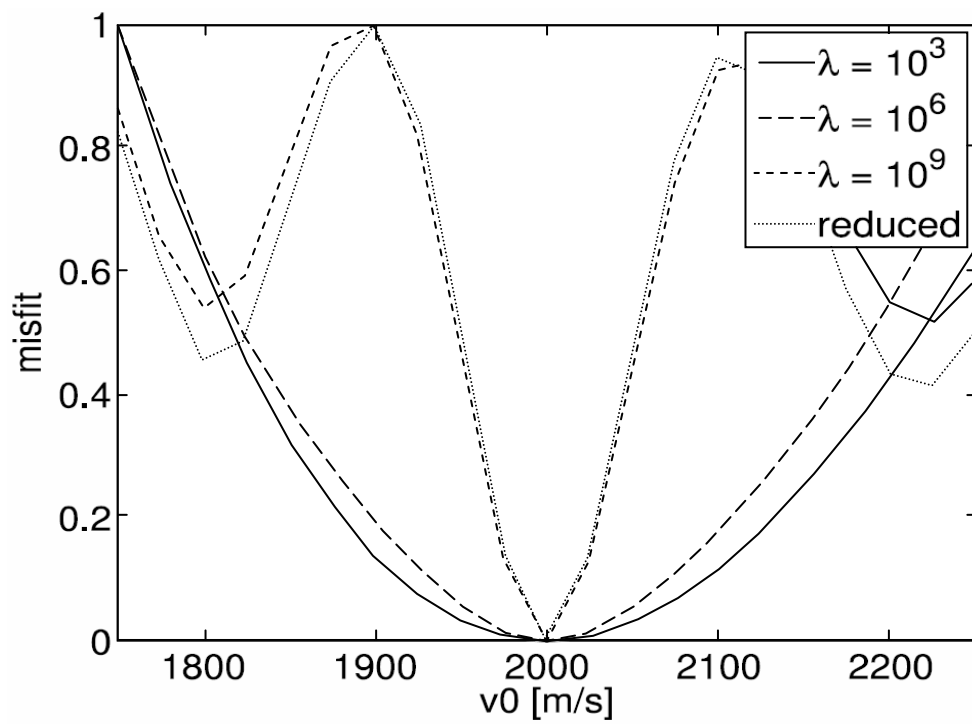
Fig.2

Fig.3

Fig.4

Fig.5

Fig.6

Fig.7

Fig.8

Fig.9

Fig.10

Fig.11

Fig.12

Fig.13

Fig.14