The representer method for state and parameter estimation in single-phase Darcy flow

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Abstract

The objective of this paper is to study the representer method for the inverse problem of combined parameter and state estimation in single-phase Darcy flow in porous media. A variational formulation is posed for the generalized inverse problem in the sense of weighted least-squares. An iterative representer-based algorithm is derived to approximate the Euler–Lagrange equations. It is proved that the linearized problem can be solved exactly by an extension of the representer method which inherits the same well-known properties of this technique. Implementation of the numerical algorithm for synthetic numerical experiments shows improved estimates of the poorly known prior guess.

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1. Introduction

The representer method is a data assimilation technique that solves the generalized inverse problem of minimizing a weighted least-squares functional that penalizes the error misfit in measurements and model dynamics. For some applications, it has been proved [4] that the search space for the minimum of the cost functional is generated by a finite number of “representer” functions that depend on the model dynamics and the corresponding measurement functional. The minimum of the least-squares problem is reduced to the solution of a linear system that allows one to define the solution as a linear combination of the “representers”.

The representer method has been successfully implemented in oceanography and meteorology [4,5] where several validations have already been performed. For reservoir applications, new technologies for data collection are becoming available and it is of interest to apply data assimilation methods to this field. Baird and Dawson [2,3] have recently introduced and studied the representer method for single-phase Darcy flow in porous media assuming perfect knowledge of the permeability field. However, it is also of particular importance to include the parameter estimation of reservoir properties into the data assimilation problem. In this case, even if the dynamics of the problem are linear, the parameter estimation becomes strongly nonlinear.

Several publications [1,12] have studied the implementation of the Ensemble Kalman Filter for continuously updating reservoir model properties by assimilating measured data. This technique is easy to implement although its accuracy depends on the size of the ensemble under consideration. Computational cost for the simulation may increase with the size of the ensemble. Variational techniques have been proposed for the parameter estimation problem, and a few recent papers describe the representer method for the approximation of the inverse solution. For example, Eknes and Evensen [6] studied parameter estimation in an Ekman model with an iterative algorithm that computes at each iteration the state and adjoint
variable with the representer method, while the parameters are computed with a gradient descent method. For inverse groundwater modeling, Valstar [10,11] derived a representer-based algorithm which introduces an extra representer for the parameter update.

In this paper, we study data assimilation in single-phase Darcy flow in porous media. In Section 2, we define the general inverse problem in the case of poorly known permeability. We assume the measurements are formulated as linear functionals. The model dynamics are a weak constraint for the inverse problem of state and parameter estimation. The adopted variational approach is a weighted least-squares where the weights are defined as the inverse of the prior covariances. In [7] we showed that these covariances play an important role in the inverse problem because they determine the smoothness of the solution to the Euler–Lagrange (EL) equations (the generalized inverse). In fact, based on the regularity of the prior error statistics, model dynamics and measurement functionals, we have shown [7] the local existence of the solution to the EL equations. This system of equations is nonlinear and an iterative scheme is proposed to approximate a solution. In Section 3, we linearize the model equations with a first order approximation around a forward model defined for each level of the iteration in terms of previous estimates. The linearized inverse problem is solved with the representer method including an extra representer set of functions for the parameter estimate as defined in [10]. In Section 4, we discuss the geometrical formulation of the representer method for the linearized parameter estimation problem. We also formally provide some results to justify that for the single-phase flow model, the representer method is a solution to the linearized problem. It is also shown that the same structure is inherited for the classical representer method and a discussion about posterior error estimates is provided. Finally, in Section 5 we present two synthetic examples where the numerical algorithm was tested. We study the case of a two-dimensional data assimilation where both the model and the parameter are inverted. Numerical experiments show that this algorithm generates an inverse solution and a parameter estimate that considerably improves the solution.

2. Generalized inverse formulation

The dynamical problem we consider is single-phase compressible flow through porous media in a domain $\Omega \subset \mathbb{R}^n$, $n \geq 2$, having a boundary consisting of two disjoint parts $\Gamma_N$ and $\Gamma_D$. The system is governed by

\[
\frac{\partial p}{\partial t} - \nabla \cdot (K \nabla p) = F \quad \text{in} \quad \Omega \times (0,T],
\]

\[
p = I \quad \text{in} \quad \Omega \times \{0\},
\]

\[
K \nabla p \cdot n = B_N \quad \text{on} \quad \Gamma_N \times (0,T],
\]

\[
p = B_D \quad \text{on} \quad \Gamma_D \times (0,T],
\]

where $p(x,t)$ is the pressure, $c$ the constant compressibility factor, $F$ the forcing function, $I$ the initial pressure, and $B_N$ and $B_D$ are the Neumann and Dirichlet boundary conditions, respectively. $K$ is a symmetric positive definite matrix that describes the permeability of the medium. In practice, functions $F$, $I$, $B_N$, $B_D$ and $K$ may not be known accurately or they may not even be available pointwise in the domain. With only poorly known available data, system (2.1)–(2.4) is called the “forward model” and its solution is a pressure field denoted by $p_F$. In general, $p_F$ is different from the “true” pressure field $p_T$ obtained from (2.1)–(2.4) if the model (i.e. functions $F$, $I$, $B_N$, $B_D$ and $K$) were perfectly known.

For any pressure field $p(x,t)$, the measurement (observation) process is defined mathematically by

\[
\mathcal{L}_m(p) = \int_0^T \int_\Omega H_m(x,t)p(x,t) d\Omega dt, \quad \text{for} \quad m = 1 \ldots M,
\]

for prescribed functions $\{H_1, \ldots, H_m\}$.

Assume there is a vector of $M$ measurements $d = (d_1, \ldots, d_M)^T$ taken from $p_T$. These measurements are allowed to contain errors due to an imperfect measuring device, for example. In other words,

\[
d = \mathcal{L}'(p_T) + \epsilon,
\]

where $\epsilon$ is a vector of measurement errors and $\mathcal{L}'(p_T) = (\mathcal{L}'_1(p_T), \ldots, \mathcal{L}'_M(p_T))$.

In order to characterize the true model let us assume that there exist functions $f, i, b_N, b_D$ and $k$ such that the true pressure field is given by the solution to the following system

\[
c \frac{\partial p}{\partial t} - \nabla \cdot (K \nabla p) = F + f \quad \text{in} \quad \Omega \times (0,T],
\]

\[
p = I + i \quad \text{in} \quad \Omega \times \{0\},
\]

\[
K \nabla p \cdot n = B_N + b_N \quad \text{on} \quad \Gamma_N \times (0,T],
\]

\[
p = B_D + b_D \quad \text{on} \quad \Gamma_D \times (0,T],
\]

\[
K = \bar{K} + k \quad \text{on} \quad \Omega.
\]

For example, $f$ is the error of the forcing term between the true and the forward model. In general, the error functions added to the prior data are the evidence of inherent uncertainty in the problem under consideration. They could be defined as random fields with a specified covariance and mean. For this analysis, the error functions involved in the previous system are viewed as deterministic control variables. Nevertheless, in the formulation we assume that there are previously defined error covariance functions (symmetric and positive definite) $C_F, C_I, C_N, C_D$ and $C_k$ related to the error functions $f, i, b_N, b_D$ and $k$, respectively. Finally, the true solution is completely characterized if we consider Eq. (2.6) where the measurement error is assumed to have a covariance matrix denoted by $W^{-1}$.

Suppose now we are given prior functions (the best available to us) $F$, $I$, $B_N$, $B_D$ and $K$ that uniquely define...
the solution to the forward model. It is clear that \( p_F \) in general will not agree with prescribed data. On the other hand, finding the true solution is not possible since the error functions are unknown. Then, the problem is to find a generalized inverse as a pressure field providing the best fit to the model and data. The strategy is based on the minimization of a weighted least-squares functional. We expect the minimum to be a set of error functions \( f, i, b_N, b_D \) and \( k \) such that the generalized inverse solution \( \hat{p} \) of (2.7)–(2.11) will be the best fit to the measurements.

For clarity in the notation, given two arbitrary functions \( f \) and \( g \), we define the following operations:

\[
\begin{align*}
  f \bullet g &= \int_0^T dt \int \Omega dx \{ f(x, t)g(x, t) \}, \\
  f \circ g &= \int_\Omega dx \{ f(x)g(x) \}, \\
  f \ast g &= \int_0^T dt \int_{\mathcal{T}} ds \{ f(s, t)g(s, t) \}, \\
  f \ast g &= \int_0^T dt \int_{\mathcal{T}} ds \{ f(s, t)g(s, t) \}.
\end{align*}
\]

It is assumed that in each case the domain of \( f \) and \( g \) is defined according to the domain of integration.

We denote by \( W \) the inverse of the measurement error covariance matrix. Furthermore, let \( W_F \) be the formal inverse of \( C_F \) [9, Chapter 7] which is also a symmetric positive function such that

\[
W_F(x, t, x', t') = \delta(x - x')\delta(t - t').
\]  

(2.12)

With similar definitions for \( W_I, W_N, W_D \) and \( W_K \), we define now a weighted least-squares cost functional

\[
\mathcal{J}[f, i, b_N, b_D, k] = (d - \mathcal{L}(p))^TW(d - \mathcal{L}(p)) + f \circ W_F \circ f + i \circ W_I + N \]

\[
+ b_N \star W_N \star b_N + b_D \star W_D \star b_D + k \circ W_K \circ k,
\]  

(2.13)

that penalizes the mismatch between observations and model error functions. The inverse problem is to find a minimum of (2.13) such that \( p \) satisfies (2.7)–(2.11). With a stochastic approach, when the dynamics are linear and the prior errors are assumed Gaussian, the least-squares functional is equivalent to the Bayesian maximum likelihood estimator [9]. For nonlinear problems the least-squares functional can be related to a best linear unbiased estimator. Therefore, the definition of the penalty functional is established in connection with other mathematical techniques to study inverse problems. For practical applications the weights may be difficult to find although they are not essential for the implementation as will be shown in the following sections.

It is important to mention that for the correct physical interpretation as well as for existence and uniqueness of the model solution, the permeability tensor \( K \) has to be positive definite. Eq. (2.11) has to be provided with an hypothesis on both \( K \) and \( k \) so that this requirement is fulfilled. In the rest of this document we will consider the case where \( k \) is an isotropic field that can be written as \( kI \), where \( I \) is the identity matrix. For this case, the aforementioned requirement implies that \( k \) has to be positive. In numerical applications, pseudo-random fields are usually needed to test the capability of the inverse technique for estimating permeability. The corresponding covariance function has to be adequately selected to prevent the generated field from having nonpositive values. However, if a permeability field is not positive at some point of its domain, the entire field must be totally discarded from the experiment.

3. The Euler–Lagrange equations

We point out that the penalty functional was defined in terms of weight functions. However, in practice we might be given information only in terms of prior error covariances (formal inverses of weights). Expressions and regularity for the weights may not be available and then nothing can be said a priori about the existence of a global minimizer. Moreover, even if a global minimizer exits, it may not be unique since the functional \( J \) is not in general convex. Having expressions for the prior error covariances, we can attempt to find a minimizer by solving the EL equations that in general ensure the existence of an extremum. In [7] we showed that the necessary condition for an extremum of \( J \) gives rise to the following system of nonlinear EL equations:

\[
- c \frac{\partial \lambda}{\partial t} - \nabla \cdot (K \nabla \lambda) = (d - \mathcal{L}(p))W \quad \text{in} \quad \Omega \times (0, T],
\]

(3.1)

\[
c \lambda = 0 \quad \text{in} \quad \Omega \times \{ T \},
\]

(3.2)

\[
K \nabla \lambda \cdot n = 0 \quad \text{on} \quad \Gamma_N \times (0, T],
\]

(3.3)

\[
\lambda = 0 \quad \text{on} \quad \Gamma_D \times (0, T].
\]

(3.4)

State:

\[
- c \frac{\partial p}{\partial t} - \nabla \cdot (K \nabla p) = F + C_F \lambda \quad \text{in} \quad \Omega \times (0, T],
\]

(3.5)

\[
p = I + C_I c \lambda \quad \text{in} \quad \Omega \times \{ 0 \},
\]

(3.6)

\[
K \nabla p \cdot n = B_N + C_N \kappa \quad \text{on} \quad \Gamma_N \times (0, T],
\]

(3.7)

\[
p = B_D - C_D \kappa \quad \text{on} \quad \Gamma_D \times (0, T].
\]

(3.8)

Parameter:

\[
K = \mathcal{K} - C_K \int_0^T \nabla \lambda \cdot \nabla p dt.
\]

(3.9)

In Eq. (3.1) we have defined the vector \( H = (H_1(x, t), \ldots, H_M(x, t)) \). We remark that Eqs. (3.1)–(3.8) are the same EL equations that were derived in [3] for Dirac delta weights and for fixed permeability \( K \). Here we have an additional equation corresponding to the parameter that makes the problem nonlinear. In [7] we proved that under some regularity conditions for the prior error covariances,
the forward model and the measurement functionals, the EL equations have a local solution (the generalized inverse).

3.1. Linearization

The coupled set of nonlinear EL equations derived in the previous section is going to be approximated by an iterative numerical algorithm. An initial guess is used to initialized the algorithm and updates are computed by solving a linearized version of the EL equations. There are several possible linearizations of the EL equations that may be found in the literature [5, Section 3.3.3]. In this document we take a first order approximation to problem (2.7)-(2.11) around an updated forward model determined by previous estimates. The linearized forward model is used to define the generalized inverse problem at each iteration step. The EL equations are derived for this linear problem and solved exactly by the representor method. Consider the operator

\[ G(p, K) = \begin{bmatrix} c \frac{\partial p}{\partial t} - \nabla \cdot (K \nabla p) \\ p|_{t=0}^n \\ Kn p \cdot n|_{\Gamma_N} \\ p|_{\Gamma_D}^n \\ K \end{bmatrix}. \] (3.10)

Note that a solution of the forward model (2.1)-(2.4) can be read as

\[ G(p_F, K) = [F, I, B_N, B_D, K]^T. \] (3.11)

For \( n = 1 \) we define the initial guess of the algorithm as \( K_0 = K, F_0 = F, p_0 = I, B_D^0 = B_D \) and \( B_N^0 = B_N \). At the \( n \)-th step the \( n \)-th forward model is defined by the solution to

\[ \frac{\partial p_n^m}{\partial t} - \nabla \cdot (K_n^{-1} \nabla p_n^m) = F_n^{-1}, \quad \text{in} \ \Omega \times (0, T], \] (3.12)

\[ p_n^m = I_n^{-1}, \quad \text{in} \ \Omega \times \{0\}, \] (3.13)

\[ K_n^{-1} \nabla p_n^m \cdot n = B_N^0, \quad \text{on} \ \Gamma_N \times (0, T], \] (3.14)

\[ p_n^m = B_D^0, \quad \text{on} \ \Gamma_D \times (0, T]. \] (3.15)

Assuming that \( p_n^m - p_F^m \) and \( K_n - K_n^{-1} \) are sufficiently small, the first order approximation of \( G \) around the \( n \)-th forward model is computed

\[ G(p_n^m, K^m) \approx G(p_F^m, K^m) + DG(p_F^m, K^m) \begin{bmatrix} p_n^m - p_F^m \\ K_n - K_n^{-1} \end{bmatrix}, \] (3.16)

where \( DG(p, K) \) is the Frechet derivative of \( G \):

\[ DG(p, K) \begin{bmatrix} \hat{p} \\ \hat{K} \end{bmatrix} = \begin{bmatrix} c \frac{\partial \hat{p}}{\partial t} - \nabla \cdot (K \nabla \hat{p}) - \nabla \cdot (\hat{K} \nabla p) \\ \hat{p}|_{t=0}^n \\ (\hat{K} \nabla p \cdot n + K \nabla \hat{p} \cdot n)|_{\Gamma_N} \\ \hat{p}|_{\Gamma_D}^n \\ \hat{K} \end{bmatrix}. \] (3.17)

From the definition of \( p_F^m \) (3.12)-(3.15) it follows that

\[ G(p, K) \approx \begin{bmatrix} c \frac{\partial p}{\partial t} - \nabla \cdot (K_n^{-1} \nabla p) - \nabla \cdot (K - K_n^{-1}) \nabla p_F^m \\ p|_{t=0} \\ (K_n^{-1} \nabla p \cdot n + (K - K_n^{-1}) \nabla p_F^m \cdot n)|_{\Gamma_N} \\ p|_{\Gamma_D} \\ K \end{bmatrix}. \] (3.18)

and obviously

\[ G(p_F^m, K_n^{-1}) \approx [F_n^{-1}, I_n^{-1}, B_D^{-1}, B_N^{-1}, K_n^{-1}]^T. \] (3.19)

It is notable that for each iteration the computation of the forward model is based on previous estimates. From (3.18) we note that linear model dynamics are governing the problem and since the actual data \( d \) is also available at each iteration step, we may apply the argument in Section 2 to define a generalize inverse problem at this level. For this purpose consider functions \( f^a, f^b, b_n^a, b_D^a \) and \( k^a \) to account for uncertainty and suppose the true solution (from which data is available) can be written as the solution of

\[ G(p, K) \approx [F_n^{-1} + f_n, I_n^{-1} + f_n, B_D^{-1} + b_D^a, B_N^{-1} + b_N^a, \]

\[ B_D^{-1} + b_D^a + b_D^a + b_N^a + k^a] \cdot \] (3.20)

This inverse problem is solved by defining the \( n \)-th penalty functional \( f^a \)

\[ f^a[p, K] = (d - \mathcal{L}(p))^T \mathbf{W} (d - \mathcal{L}(p)) + f_n \cdot W_F \cdot f_n \]

\[ + f_n \circ W_D \circ f_n + b_N^a \cdot W_N \cdot b_N^a \]

\[ + b_D^a \cdot W_D \cdot b_D^a + k^a \circ W_K \cdot k^a. \] (3.21)

The EL equations for this linear inverse problem are the following:

State:

\[ c \frac{\partial p^a}{\partial t} - \nabla \cdot (K_n^{-1} \nabla p^a) - \nabla \cdot (K - K_n^{-1}) \nabla p_F^m = F_n^{-1} + C_F \cdot z^a \quad \text{in} \ \Omega \times (0, T], \] (3.22)

\[ p^a = I_n^{-1} + C_I \cdot c z^a \quad \text{in} \ \Omega \times \{0\}, \] (3.23)

\[ K_n^{-1} \nabla p^a \cdot n + (K_n - K_n^{-1}) \nabla p_F^m \cdot n = B_N^{-1} + C_N \cdot z^a \quad \text{on} \ \Gamma_N \times (0, T], \] (3.24)

\[ p^a = B_D^{-1} - C_D \cdot K_n^{-1} \nabla z^a \cdot n \quad \text{on} \ \Gamma_D \times (0, T]. \] (3.25)

Adjoint:

\[ - c \frac{\partial z^a}{\partial t} - \nabla \cdot (K_n^{-1} \nabla z^a) = (d - \mathcal{L}(p_n^m))^T \mathbf{WH} \quad \text{in} \ \Omega \times (0, T], \] (3.26)

\[ c z^a = 0 \quad \text{in} \ \Omega \times \{T\}, \] (3.27)

\[ K_n^{-1} \nabla z^a \cdot n = 0 \quad \text{on} \ \Gamma_N \times (0, T], \] (3.28)

\[ z^a = 0 \quad \text{on} \ \Gamma_D \times (0, T). \] (3.29)

Parameter:

\[ K_n = K_n^{-1} - C_K \int_0^T \nabla z^a \cdot \nabla p_F^m. \] (3.30)
From the EL equations we consider the following updates for the forcing, initial and boundary conditions
\[ F^n = F^{n-1} + C_F \bullet \zeta^n, \]  
\[ I^n = I^{n-1} + C_I \circ c \zeta^n, \]  
\[ B_{N}^n = \nabla I^{n-1} + C_N \star \zeta^n, \]  
\[ B_{D}^n = B_{D}^{n-1} - C_D \star K^{n-1} \nabla \zeta^n. \]  
(3.31) (3.32) (3.33) (3.34)

In the following section we discuss the representor method for the solution to the linearized problem (3.22)–(3.30).

4. The representor method

4.1. Motivation

We proceed formally to show the idea behind the representor method for solving the linearized inverse problem arising at each step of the iteration. For simplicity, only Neumann boundary conditions are considered \((\Gamma = \Gamma_N\) and \( I_D = \emptyset \)). After the \((n-1)\)th step of the algorithm, an update \((K^{n-1}, F^{n-1}, I^{n-1}, B_{N}^{n-1})\) is generated and an \(n\)th forward model can be computed by (3.12)–(3.14). We now recall that the prior error covariances are assumed to be positive definite. Then, it is possible to find the square root in the sense of [9, Chapter 7], that is
\[ C_F^\frac{1}{2}(x,t,x',t') \bullet C_F^\frac{1}{2}(x',t',x,t') = C_F(x,t,x',t'). \]  
(4.1)

For a better description of the spaces and the regularity conditions for the prior error covariances we refer the reader to [7]. For this analysis it is enough to define the following spaces
\[ X \equiv \{ K \in C^{1,\frac{1}{2}}(\Omega) : \zeta \in K(x) \text{ for all } x \in \Omega \} \]  
(4.2)

where \( \zeta \) is a positive constant and
\[ \mathcal{P}^n \equiv \{ p \in H^{1,\frac{1}{2}}(\Omega) \mid p \text{ is solution of } (4.4)-(4.7) \text{ for some } (f,i,b_N,k) \}, \]  
(4.3)

where
\[ \frac{d p}{dt} - \nabla \cdot (K^{n-1} \nabla p) - \nabla \cdot (K \nabla p_F^n) = C_F^\frac{1}{2} \bullet f \]  
in \( \Omega \times (0,T) \),  
(4.4)

\[ p = C_I^\frac{1}{2} \circ i \]  
in \( \Omega \times \{0\} \),  
(4.5)

\[ K^{n-1} \nabla p \cdot n + K \nabla p_F^n \cdot n = C_k^\frac{1}{2} * b_N \]  
on \( \Gamma \times (0,T) \),  
(4.6)

\[ K = C_k^\frac{1}{2} \circ k \]  
on \( \Omega \times \{0\} \).  
(4.7)

It is not difficult to see [7, Lemma 1] that those terms in the right hand side of (4.4)–(4.7) are as smooth as the square root of the covariances. Therefore, we may assume formally that the square root covariances are smooth enough such that for any combination of
\[ (f,i,b_N,k) \in L^2(0,T;L^2(\Omega)) \times L^2(\Omega) \times L^2(0,T;L^2(\Gamma)) \times L^2(\Omega), \]  
(4.8)

problem (4.4)–(4.7) admits a unique solution in \( \mathcal{P}^n \times X \). We now formally define the following operator on \( \mathcal{P}^n \times X \):
\[ A^n(p,K) = \begin{bmatrix} A^n_1(p,K) \\ A^n_2(p,K) \\ A^n_3(p,K) \\ A^n_4(p,K) \end{bmatrix} \]  
(4.9)

and a bilinear form is defined on \([\mathcal{P}^n \times X]_2^2\) as
\[ B^n[(p_1,K_1), (p_2,K_2)] = A^n_1(p_1,K_1) \bullet W_F \bullet A^n_2(p_2,K_2) \]  
\[ + A^n_3(p_1,K_1) \circ W_I \circ A^n_4(p_2,K_2) \]  
\[ + A^n_5(p_1,K_1) \star W_N \star A^n_6(p_2,K_2) \]  
\[ + A^n_7(p_1,K_1) \circ W_K \circ A^n_8(p_2,K_2). \]  
(4.10)

With this definition, the \(n\)th penalty functional (3.21) is written in the following way
\[ J^n[p,K] = B^n[(p - p_F^n, K - K^{n-1}), (p - p_F^n, K - K^{n-1})] \]  
\[ + (d - \mathcal{L}(p))W(d - \mathcal{L}(p)). \]  
(4.11)

Recalling that \( W_F, W_I, W_N \) and \( W_K \) are assumed symmetric positive definite, we have the following:

Lemma 4.1. \( B^n \) is an inner product on \( \mathcal{P}^n \times X \).

Proof. Since \( B^n \) is symmetric and the weights are positive definite, \( B^n \) is positive semidefinite. We need to show only that \( B^n[(p,K), (p,K)] = 0 \) implies \( (p,K) = (0,0) \). Assume \( B^n[(p,K), (p,K)] = 0 \) for some \((p,K) \in \mathcal{P}^n \times X \). This means that there exists functions \( f, i, b_N, K \) such that \( p, K \) solves:
\[ \frac{d p}{dt} - \nabla \cdot (K^{n-1} \nabla p) - \nabla \cdot (K \nabla p_F^n) = C_F^\frac{1}{2} \bullet f \]  
in \( \Omega \times (0,T) \),  
(4.12)

\[ p = C_I^\frac{1}{2} \circ i \]  
in \( \Omega \times \{0\} \),  
(4.13)

\[ K^{n-1} \nabla p \cdot n + K \nabla p_F^n \cdot n = C_k^\frac{1}{2} * b_N \]  
on \( \Gamma \times (0,T) \),  
(4.14)

\[ K = C_k^\frac{1}{2} \circ k \]  
on \( \Omega \times \{0\} \).  
(4.15)

On the other hand, \( B^n[(p,K), (p,K)] = 0 \) yields
\[ A^n_1(p,K) \bullet W_F \bullet A^n_2(p,K) + A^n_3(p,K) \circ W_I \circ A^n_4(p,K) \]  
\[ + A^n_5(p,K) \star W_N \star A^n_6(p,K) + A^n_7(p,K) \circ W_K \circ A^n_8(p,K) \]  
\[ = 0. \]  
(4.16)

From the definition of \( A^n \) (4.9) and using the fact that \((p,K)\) solves (4.12)–(4.15), the previous expression implies
\[ ||f||_{L^2(0,T;L^2(\Omega))} + ||i||_{L^2(\Omega)} + ||b_N||_{L^2(\Gamma)} + ||k||_{L^2(\Omega)} = 0. \]  
(4.17)
Then \( f = 0, i = 0, b_N = 0 \) and \( k = 0 \) (in the sense of (4.8)). Directly from (4.15) it follows \( K = 0 \) and from (4.12)-(4.14) we see that \( p \) is the weak solution of a parabolic equation with zero forcing, zero initial condition and zero boundary data. It follows from standard techniques [8, Chapter 4] that \( \| p \|_{\mathcal{L}^2(\Omega_T)} \leq 0 \) which in turn implies \( p = 0 \) in \( \mathcal{P} \). Therefore, \( \mathcal{B}^n \) defines an inner product on \( \mathcal{P} \times \mathcal{K} \). \( \square \)

**Theorem 1.** \( \mathcal{P} \times \mathcal{K} \) is a Hilbert-Space with the inner product given by

\[
\mathcal{B}^n((p_1, K_1), (p_2, K_2)) = \langle (p_1, K_1), (p_2, K_2) \rangle. \tag{4.18}
\]

**Proof.** We take a Cauchy sequence in \( \mathcal{P} \times \mathcal{K} \) with respect to \( \langle , \rangle \) defined above. By definition of \( \mathcal{P} \) there are sequences \( f_m, l_m, b_N^m \) and \( k_m \) such that, for all \( m \),

\[
\frac{\partial p_m}{\partial t} - \nabla \cdot (K_m \nabla p_m) - \nabla \cdot (K_m \nabla p_m^f) = C_{F} \cdot f_m \quad \text{in } \Omega \times (0, T), \quad \tag{4.19}
\]

\[
p_m = C_{K}^1 \cdot i_m \quad \text{in } \Omega \times \{0\}, \quad \tag{4.20}
\]

\[
K_m \nabla p_m \cdot \mathbf{n} + K_m \nabla p_m^f \cdot \mathbf{n} = C_{N}^m + b_N^m \quad \text{on } \Gamma \times (0, T), \quad \tag{4.21}
\]

\[
K_m = C_{K}^1 \cdot k_m \quad \text{in } \Omega \times \{0\}. \quad \tag{4.22}
\]

Note that for all \( m \) and \( j \)

\[
\| (p_m - p_j, K_m - K_j) \|_{\mathcal{P} \times \mathcal{K}} \leq \langle (p_m - p_j, K_m - K_j) \rangle = \langle f_m - f_j, l_m - l_j \rangle + \| i_m - i_j \|_{\mathcal{L}^2(\Omega)} + \| b_N^m - b_N^j \|_{\mathcal{L}^2(\Gamma_T)} + \| k_m - k_j \|_{\mathcal{L}^2(\Omega)} \quad \tag{4.23}
\]

Since \( (p_m, K_m) \) is Cauchy with respect to \( \langle , \rangle \), as \( m, j \to \infty \), the last expression goes to zero which means that each term of the right hand side goes to zero. Then \( f_m, l_m, b_N^m \) and \( k_m \) are Cauchy sequences in \( L^2(0, T; L^2(\Omega)) \), \( L^2(\Omega) \), \( L^2(0, T; L^2(\Gamma)) \) and \( L^2(\Omega) \), respectively. By completeness we choose \( f^*, i^* \), \( b_N^* \) and \( k^* \) which are limits of those sequences in the corresponding spaces. From the assumption of smooth square root covariances, as we already remarked [7, Lemma 1] the right hand side of (4.4)-(4.7), for \( f^*, i^*, b_N^* \) and \( k^* \) is smooth enough to generate an admissible solution \( (p^*, K^*) \in \mathcal{P} \times \mathcal{K} \). Moreover,

\[
\| (p^* - p_m, K^* - K_m) \|_{\mathcal{P} \times \mathcal{K}} = \| f^* - f_m \|_{L^2(0, T; L^2(\Omega))} + \| i^* - i_m \|_{L^2(\Omega)} + \| b_N^* - b_N^m \|_{L^2(\Gamma_T)} + \| k^* - k_m \|_{L^2(\Omega)} \quad \tag{4.24}
\]

and therefore as \( m \to \infty \), \( (p_m, K_m) \to (p^*, K^*) \) with the norm induced by \( \langle , \rangle \) and we have proved the result. \( \square \)

**Corollary 1.** If the measurement functional \( \mathcal{L} \) defined in (2.5) is continuous in \( H^2(\Omega_T) \), then it is continuous with respect to \( \langle , \rangle \).
and from (3.31)
$$\mathscr{J}^\eta[p, K] = \sum_{m,j=1}^M b_n b_j \mathcal{L}^\eta(p_m) + \langle (p^*, K^*), (p^*, K^*) \rangle + (d - \mathcal{L}^\eta(p))^\top \mathbf{W}(d - \mathcal{L}^\eta(p)). \tag{4.35}$$

Also from (3.31) we may obtain
$$\mathcal{L}^\eta(p) = \langle (p, K), (\rho_m, \mu_m) \rangle = \langle (p^*, K^*), (p^*, K^*) \rangle + \sum_{j=1}^M b_j \langle (\rho_j, \mu_j), (\rho_m, \mu_m) \rangle = \mathcal{L}^\eta(p_m) + b_j \mathcal{L}^\eta(p_j). \tag{4.36}$$

Defining the matrix $\mathbf{R}$ so that $R_{m,j} = \mathcal{L}^\eta(p_j)$, we conclude that
$$\mathcal{L}^\eta(p) = \mathcal{L}(p^\eta) + \mathbf{Rb}. \tag{4.37}$$

Then,
$$\mathscr{J}^\eta[p, K] = \mathbf{b}^\top \mathbf{R} \mathbf{b} + \langle (p^*, K^*), (p^*, K^*) \rangle \tag{4.38}$$
$$+ (d - \mathcal{L}(p^\eta) - \mathbf{Rb})^\top \mathbf{W}(d - \mathcal{L}(p^\eta) - \mathbf{Rb}). \tag{4.39}$$

If $(p, K)$ minimizes $\mathscr{J}^\eta$, then
$$\langle (p^*, K^*), (p^*, K^*) \rangle = 0. \tag{4.40}$$

From the definition of $\mathscr{J}^\eta$ and $\langle \cdot \rangle$ we have that $p^* = 0$ and $K^* = 0$. Therefore, the minimization of $\mathscr{J}^\eta$ is reduced to the minimization of
$$\mathscr{J}^\eta = \mathbf{b}^\top \mathbf{R} \mathbf{b} + (d - \mathcal{L}(p^\eta) - \mathbf{Rb})^\top \mathbf{W}(d - \mathcal{L}(p^\eta) - \mathbf{Rb}). \tag{4.41}$$

This is exactly the same expression in [4, Chapter 5, (5.5.13)]. There, it is shown that the optimum for $\mathbf{b}$ is given by
$$(\mathbf{R} + \mathbf{W}^{-1}) \hat{\mathbf{b}} = \mathbf{d} - \mathcal{L}(p^\eta). \tag{4.42}$$

We have shown that the solution to the linearized minimization problem can be expressed in terms of a finite linear combination of functions where the coefficients are the solution to the finite-dimensional system (4.42). Finally, the same argument used in [4, Chapter 5, (5.5.13)] shows that for the optimum,
$$\mathscr{J}^\eta = (d - \mathcal{L}(p^\eta)) (\mathbf{R} + \mathbf{W}^{-1})^{-1} (d - \mathcal{L}(p^\eta)). \tag{4.43}$$

5. Implementation

In this section, we derive an algorithm that computes an update $(p^\eta, L^\eta, K^\eta)$ which we expect to be a good approximation of the original EL equations. At the nth iteration we are given $K^{n-1}, F^{n-1}, F_m^{n-1}, B_m^{n-1}, B_m^{n-1}$. After computing the nth forward model solution $p^\eta$, the linearized problem (3.22)–(3.30) is solved by the representer method. If there is evidence that the forward model itself is close enough to the true model, we conclude that convergence is achieved since there is not enough information (except noise) to continue the inversion. The problem is now to solve the linearized EL equations. From the previous section we may assume that the solution can be written as a linear combination of $M$ “representer” functions to be determined. Assume that
$$L^n = \sum_{m=1}^M b^\alpha_m z^\alpha_m, \tag{5.1}$$
$$p^n = p^\eta + \sum_{m=1}^M b^\eta_m z^\eta_m, \tag{5.2}$$
$$K^n = K^{n-1} + \sum_{m=1}^M b^\gamma_m z^\gamma_m, \tag{5.3}$$

where $z^\alpha_m, r^\alpha_m, z^\gamma_m$ are the adjoint, state and parameter representers, respectively, and $b^\alpha_m$ are the representers coefficients. In (5.3) we note the extra representer for the parameter unknown as also used in [10]. If we substitute the expression (5.1) into (3.26)–(3.29) we obtain that each adjoint representer $z^\alpha_m$ satisfies
$$-c \frac{\partial z^\alpha_m}{\partial t} - \nabla \cdot (K^{n-1} \nabla z^\alpha_m) = H_m \quad \text{in } \Omega \times (0, T], \tag{5.4}$$
$$cz^\alpha_m = 0 \quad \text{in } \Omega \times \{0\}, \tag{5.5}$$
$$K^{n-1} \nabla z^\alpha_m \cdot n = 0 \quad \text{on } \Gamma_N \times (0, T], \tag{5.6}$$
$$z^\alpha_m = 0 \quad \text{on } \Gamma_D \times (0, T), \tag{5.7}$$

where the representers coefficients are given by
$$b^\alpha_m = \sum_{mj} (d_i - \mathcal{L}_i(p^\eta)) W_{mj}, \tag{5.8}$$
or
$$\mathbf{b}^\alpha = \mathbf{W}(d - \mathcal{L}(p^\eta)). \tag{5.9}$$

Next we substitute the expressions (5.1) and (5.3) into (3.22)–(3.25) to find that each parameter representer $z^\gamma_m$ satisfies
$$z^\gamma_m = -C_K \int_0^T \nabla z^\alpha_m \cdot \nabla p^\eta \tag{5.10}$$

Substituting (5.2) and (5.3) into expression (3.30) and using (3.12)–(3.15) we directly find that the state representer $r^\eta_m$ is the solution to the problem
$$c \frac{\partial r^\eta_m}{\partial t} - \nabla \cdot (K^{n-1} \nabla r^\eta_m) - \nabla \cdot (z^\gamma_m \nabla p^\eta) = C_F \star z^\gamma_m \quad \text{in } \Omega \times (0, T], \tag{5.11}$$
$$r^\eta_m = C_N \star z^\gamma_m \quad \text{in } \Omega \times \{0\}, \tag{5.12}$$
$$K^{n-1} \nabla r^\eta_m \cdot n = -z^\gamma_m \nabla p^\eta \cdot n + C_N \star z^\gamma_m \quad \text{on } \Gamma_N \times (0, T], \tag{5.13}$$
$$r^\eta_m = -C_D \star (K^{n-1} \nabla z^\alpha \cdot n) \quad \text{on } \Gamma_D \times (0, T]. \tag{5.14}$$

In order to compute the updated estimates (5.1)–(5.3) we need to find the actual representer coefficients. Therefore,
consider again Eq. (5.8) and note that $\beta^\phi$ is given by the actual pressure which is still unknown (and in fact also depends on $p_m^\phi$). However, if we substitute the expression (5.2) in (5.9) we find that

$$\beta^\phi = W \left( d - L \left( p_F^\phi + \sum_{k=1}^{M} \beta_k^\phi r_k^\phi \right) \right)$$

(5.15)

and since $L$ is linear, the last expression reduces to

$$W^{-1} \beta^\phi = \left( d - L(p_F^\phi) - \sum_{k=1}^{M} \beta_k^\phi L(r_k^\phi) \right),$$

(5.16)

which can be written as

$$(R^n + W^{-1}) \beta^\phi = d - L(p_F^\phi),$$

(5.17)

where the matrix $R^n$ is given by $R^n_{ij} = L_i(r_j^\phi)$. Note that, in order to update the algorithm we do not need to compute (5.1) and (5.2) and therefore, storage of the representers is not required. In fact, we may substitute expression (5.8) into the adjoint problem (3.26)-(3.29) to solve for $\lambda$. We compute $p^\phi$ and $K^m$ directly from (3.22)-(3.25) and (3.30), respectively.

**Remark 2.** It is a simple exercise to show that, for all $m \in \{1, \ldots, M\}$, $(\rho^m, \mu^m) = (p_m^\phi, \gamma_m^\phi)$ where $r_m^\phi$ and $\gamma_m^\phi$ are the solutions of (5.10) and (5.11)-(5.14), respectively, and $(\rho_m, \mu_m)$ were derived in (4.31). Then we have found a formula to compute the representers that were obtained with an abstract formulation presented in Section 4. Further, problem (4.42) is the same as (5.17) and by uniqueness of the linear finite-dimensional problem $\beta^\phi = b$. Then, a unique expression for the solution to the linear nth inverse problem is now available in terms of the representers that in turn can be calculated with the expressions presented in this section.

**Remark 3.** In the Appendix (Eq. (A.9)) it is shown that the matrix $R^n + W^{-1}$ equals the cross-covariance of the linearized model measurement misfit.

We summarized the results of this and the previous section in the following algorithm. Starting with $(p_F^0, K^0, F^0, I^0, B_N^0, B_D^0) = (p_F, K, F, I, B_N, B_D)$, some threshold $\theta$, prior error covariances and data observations, then,

**Outer Loop:** (over $n$)

**Input:** $K^{n-1}, F^{n-1}, I^{n-1}, B_N^{n-1}, B_D^{n-1}$

1. Compute the $n$th forward model ($p_F^n$) by solving (3.12)-(3.15). If $\|d - L(p_F^n)\| \leq \theta$. Stop.

### Table 1

<table>
<thead>
<tr>
<th>Experiment</th>
<th>$p_{ex}(x,y,t)$</th>
<th>$\mathcal{R}$</th>
<th>$\theta_{\infty}$</th>
<th>$\theta_L$</th>
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<tr>
<td>1</td>
<td>$\cos(2\pi \cos(\pi/2 \cos(\pi/2))$</td>
<td>4.0</td>
<td>5.577e$-3$</td>
<td>1.6e$-3$</td>
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<tr>
<td>2</td>
<td>$\cos(\pi \cos(\pi/2 \cos(\pi/2))$</td>
<td>3.0</td>
<td>1.700e$-3$</td>
<td>6.44e$-4$</td>
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<tr>
<td>3</td>
<td>$\cos(\pi \cos(\pi/2 \cos(\pi/2))$</td>
<td>3.0</td>
<td>1.700e$-3$</td>
<td>6.44e$-4$</td>
</tr>
<tr>
<td>4</td>
<td>$\cos(2\pi \cos(\pi/2 \cos(\pi/2))$</td>
<td>3.0</td>
<td>6.9e$-3$</td>
<td>1.9e$-3$</td>
</tr>
</tbody>
</table>

### Table 2

<table>
<thead>
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<th>Experiment</th>
<th>$\sigma_F^2$</th>
<th>$\sigma_K^2$</th>
<th>$\sigma_N^2$</th>
<th>$\sigma_{t}^2$</th>
<th>$r_F$</th>
<th>$r_K$</th>
<th>$r_{t}$</th>
<th>$w^{-1}$</th>
<th>$M$</th>
<th>$|\mathcal{R} - K|_F$</th>
</tr>
</thead>
<tbody>
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<td>1</td>
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<td>3.0</td>
<td>-</td>
<td>0.06</td>
<td>-</td>
<td>0.75</td>
<td>1.5</td>
<td>5.0e$-5$</td>
<td>14</td>
<td>3.904</td>
</tr>
<tr>
<td>2</td>
<td>0.2</td>
<td>1.5</td>
<td>0.01</td>
<td>-</td>
<td>1.0</td>
<td>0.9</td>
<td>-</td>
<td>5.0e$-5$</td>
<td>14</td>
<td>2.502</td>
</tr>
<tr>
<td>3</td>
<td>-</td>
<td>1.5</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.9</td>
<td>-</td>
<td>5.0e$-5$</td>
<td>14</td>
<td>2.502</td>
</tr>
<tr>
<td>4</td>
<td>-</td>
<td>3.0</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.75</td>
<td>9.0e$-4$</td>
<td>16</td>
<td></td>
<td>1.983</td>
</tr>
</tbody>
</table>

![Fig. 1. Experiment 1. Left: true permeability field. Right: inverse permeability.](image)
2. **Inner Loop** (for \(m = 1, \ldots, M\))

(2.1) Compute \(\alpha_m^n\) by solving (5.4)–(5.7).

(2.2) Compute \(\gamma_m^n\) from (5.10).

(2.3) Solve (5.11)–(5.14) to obtain \(r_m^n\).

3. Find \(\beta^n\) with (5.17).

4. Solve (3.26)–(3.29) to find \(\lambda^n\).

5. Compute \(K^n\) from (3.30).

6. Solve (3.22)–(3.25) for \(p^n\).

7. Update \(F^n, P^{-1}, B_N^{n-1}\) and \(B_D^{n-1}\) (3.31)–(3.34).

**Output:** \((p^n, \gamma^n, K^n)\).

A stopping criteria is selected for the \(n\)th forward model when the misfit between data and measurements is smaller than some threshold \(\theta\) determined for example, by the numerical error of the method applied to compute the forward model. Therefore, we are assuming that below this threshold the \(n\)th forward model is close enough to the data and there is no need to continue the inversion. If this criteria is satisfied at level \(n\), the output is given with the state and parameter of the previous step. Another criteria for determine convergence of this scheme can be defined in terms of the difference between \(p^n_F\) and \(p^n\) in some norm.

We should expect that as the forward model is closer to the observational data, the inverse and the forward model

---

Fig. 2. Experiment 1. Parameter posterior variance for \(n = 4\).

Fig. 3. Experiment 1. Time series of pressure at four different measurement locations.
should be closer too. A discussion about the cost of this algorithm may be found in [3], which for this case should be considered at each iteration.

Finally, it is important to mention that the representer method allows one to define expressions for the posterior covariance of measurements and model errors. For the linearized problem, the same formulas for the posterior error covariance of forcing, initial and boundary conditions can be derived in the same way as in [4, Chapter 3]. With the same arguments, in the Appendix A, we show that, for the inverse permeability $K^n$, the posterior error covariance is

$$ E(K^n_T(x) - K^n(x), K^n_T(x') - K^n(x')) = C^n_K(x, x') - \gamma^n(x)(R^n + W^{-1})^{-1}\gamma^n(x'), $$

(5.18)

where $\gamma^n(x) = (\gamma^n_1(x), \ldots, \gamma^n_M(x))$, $K^n_T$ is the true permeability of the linearized problem and $C^n_K$ is the prior error covariance for the $n$th problem. For this analysis we assume that $C^n_K$ is the same for each iteration step and equal to the original prior error covariance $C_K$ defined in Section 2. A similar formula to (5.18) in a discrete formulation was obtained in [10] for the parameter estimation in groundwater modeling.

6. Numerical experiments

In this section, we present four synthetic numerical experiments where the iterative scheme derived in the last section is implemented. For these experiments the domain $\Omega$ is a square with length of each side equal to two, and only Neumann boundary conditions are considered. The final time is $T = 0.5$ and the compressibility factor is constant $c = 1$ for each experiment. The sampling functional for these experiments is the evaluation at some space–time coordinates.

A continuous Galerkin approximation is used for the spatial discretization of the variational formulation. For computational purposes we used bi-quadratic shape functions on 9-node elements with an $8 \times 8$ grid. Time discretization was implemented with a Backward–Euler scheme with 40 time steps. For each experiment, the initial forward model (initial guess) is obtained by choosing functions $F$, $I$ and $B_N$ such that the exact solution ($p_{ef}$) to Eqs. (2.1)–(2.4) is

![Fig. 4. Experiment 1. Pressure profile at the observation time $t = T/4$. Top left: initial forward solution (initial guess). Top right: true solution. Bottom: inverse ($n = 4$) solution. Asterisk: measurement location.](image-url)
the function given in Table 1, with constant prior permeability \( K \), also given in the table. Convergence of the algorithm is determined using the criteria described in the previous section. More precisely we define the following thresholds,

\[
\theta_\infty = \frac{1}{2} \| p_F - p_{\text{ex}} \|_\infty, \quad \theta_{L^2} = \frac{1}{2} \| p_F - p_{\text{ex}} \|_{L^2},
\]

where \( p_F \) is the forward model computed numerically. The factor 1/2 was taken arbitrarily. In a more realistic setting where the exact forward model solution is not known, these thresholds could be determined, for example, by computing forward solutions using coarse and fine meshes to approximate the discretization error. Recall that at each outer loop of the algorithm above, we compute the \( n \)th forward model solution \( p^n_F \). If at the \( n \)th iteration \( \| d - L(p^n_F) \|_\infty > \theta_\infty \), then we compute the inverse solution \( p^n \) at step \( n \). If \( \| p^n - p^n_F \|_{L^2} \leq \theta_{L^2} \), we determine that convergence is achieved. In Table 1, we also show the convergence thresholds for each experiment.

The algorithm of the previous section was presented under the general consideration that the observational data, permeability, forcing, initial and boundary conditions are subject to errors. However, in the experiments we consider some of these cases independently. We must point out that the main goal of this paper is the analysis of the model when the permeability is poorly known. Therefore, all the experiments assume that the true permeability field is different from the prior guess. For example, in the first experiment we study a model that is subject to error in the initial condition while the rest (forcing and boundary conditions) are assumed correct. By this we mean that the true solution from which synthetic data is obtained, has the same forcing and boundary conditions as the forward model. It is worth noting that the formulation for this case is the same as before, except that in the corresponding cost functional we must omit the corresponding error functions \( f \) and \( b_N \) (See (3.21)). This new formulation is equivalent to (but not the same as) considering the equations in the algorithm with the posterior error covariances \( C_F \) and \( C_N \) equal to zero. The same idea is applied for experiment 2 where we assume error in the forcing and boundary conditions, and in experiments 3 and 4 where only the permeability is estimated.

We generated pseudo-random errors for the initial (experiment 1), forcing and boundary conditions

![Fig. 5. Experiment 1. Pressure profile at the initial time \( t = 0 \). Top left: initial forward solution. Top right: true solution. Bottom: inverse (\( n = 4 \)) solution.](image-url)
(experiment 2) and the permeability (experiments 1–3) according to the following covariances:

\[ C_F(x, x', t, t') = \sigma_F^2 \exp \left( \frac{|x - x'|^2}{r_F^2} \right) \delta(t - t'), \]
\[ C_I(x, x') = \sigma_I^2 \exp \left( \frac{|x - x'|^2}{r_I^2} \right), \]
\[ C_K(x, x') = \sigma_K^2 \exp \left( \frac{|x - x'|^2}{r_K^2} \right), \]
\[ C_N(x, x', t, t') = \sigma_N^2 \delta(x - x') \delta(t - t'), \]
\[ W^{-1} = w^{-1}I. \]

(6.2)

The generated pseudo-random errors were added to the prior fields \( F, I, B_N, K \) and the simulation produced a solution which was taken to be the “true solution” for each experiment. Finally, this solution was sampled at \( M/2 \) measurement locations at two different times \( (t = T/4 \) and \( t = 3T/4) \). Gaussian noise with mean zero and variance \( w^{-1} \) was added to these measurements. Pertinent information is presented in Table 2, where in the last column we show the \( L^2 \)-error of the true permeability function with respect to the prior guess.

From expressions (6.2) it is clear that the integrals weighted with \( C_K, C_F \) and \( C_I \) in problems (5.10)–(5.12), (3.22), (3.23) and (3.30)–(3.32) become convolutions over the domain. Although these experiments are performed with a small number of degrees of freedom, these convolutions are extremely expensive. For an efficient computation of those terms, the Fast Fourier Transform was implemented.

It is important to note that the true solution from which the measurements were taken was generated according to the covariances previously defined. They are also the same covariances used in the algorithm except for experiment 4 where the true permeability was explicitly prescribed. In other words, for experiments 1–3 the parameter deviations

Fig. 6. Experiment 1. Pressure profile at time \( t = T/2 \). Top left: initial forward solution. Top right: true solution. Bottom: inverse (\( n = 4 \)) solution.
have the distributions given by (6.2) with the corresponding parameters from Table 2. For experiment 4, the permeability deviation is defined as a step function. Although it is not assumed to have any given distribution, a prior error covariance is defined for the purpose of computing the convolution in expressions (5.10) and (3.30) of the algorithm.

The values of the variances presented in Table 2 are perhaps not realistic in the sense that they do not represent a percentage of the actual quantity for which they account. Since we are most interested in the response of this method to estimation of the parameter $K$, we choose a larger covariance for the permeability to show the power of the technique. Note for example that the variance for the permeability is large compared with the nominal value of $K$.

We apply the representer method at each iteration, using the same algorithm, grid and time step as those used to compute the initial guess. This gives us a numerical approximation to the minimizer of the cost functional associated with the linearized inverse problem. For each experiment we analyze the behavior of the prior $n$th penalty function that is defined by

$$J_n(p) = (d - \mathcal{L}(p_n))W^{-1}(d - \mathcal{L}(p^*_n)),$$

(6.4)

which is the penalty functional (3.21) evaluated at the $n$th forward model. After the inversion at level $n$, we compute the posterior penalty functional with expression (4.43).

### 6.1. Experiment 1

In Fig. 1 we present the “true permeability” used to compute the measurements, and the inverse permeability field computed using the representer method. It is clear that from an initial guess $K_0 = 4.0$, the inverse permeability shows vast improvement over the domain. Fig. 2 shows the posterior variance for the parameter estimate computed from the expression (5.18) (with $x = x'$) at the final iteration. We observe a considerable reduction of the constant prior error variance $\sigma^2_K = 3.0$. The improvement for both the parameter and the solution is quite good for the inverse estimate obtained from the algorithm, which for this experiment converged after four iterations. The time series for the $n$th inverse solution vs. the true solution at four of the measurement locations is presented in Fig. 3. Similar results are seen at the other measurement locations. As we expected, the inverse solution is the best fit to the model dynamics and the measurements. Fig. 4 compares the pressure profiles at the measurement time $t = T/4$. Improvement of the state is excellent not only at the measurement locations (asterisks) but also in the entire domain. In this experiment, the initial condition was assumed incorrect and the inverse solution at time $t = 0$ shows substantial improvement, as can be observed from Fig. 5. Finally, we present in Fig. 6 a comparison of the true and inverse pressure fields at time $T/2$, a time at which no measurements

<table>
<thead>
<tr>
<th>$n$</th>
<th>$|K^* - K_{n-1}|_{L^2(\Omega)}$</th>
<th>$J^*_n$</th>
<th>$J^n$</th>
<th>$|d - \mathcal{L}(p^*<em>n)|</em>{L^2(\Omega)}$</th>
<th>$|p^* - p^n|_{L^2(\Omega')}$</th>
<th>$|K^* - K|_{L^2}$</th>
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<td>2.901e-2</td>
<td>9.990e-4</td>
<td>9.260e-4</td>
<td>1.025</td>
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</tbody>
</table>

Experiment 1.
were taken. It is notable that the inverse solution shows global improvement.

Table 3 shows the information obtained at each iteration. In the final column we note the reduction in the $L^2$-norm of the error between the inverse and the true permeability. Note that the inverse permeability is closer than the prior to the true permeability (last column of Table 2) and we may conclude that the algorithm produces an improved parameter estimate. The inverse state and parameter estimates are approximate solutions to the EL equations. These solutions corresponds to a critical point of the cost functional. Even if the critical point is a minimum, in general the EL solutions may not coincide with the true solution (from which only the measurements were taken) except probably (if $\epsilon \approx 0$) at the measurement locations where the data assimilation is taking place. This explains why the error between the inverse and the true permeability does not go to zero. It is also worth mentioning that the forward model converges to the inverse estimate in the $L^2(L^2)$-norm. From Table 3 we finally observe that for each iteration step, the prior cost functional is minimized. Of course as the forward model approaches the data, both values must decrease. The posterior penalty
functional has a statistical interpretation that we do not attempt to study in the present case. At this point we note there is a decrease from the prior to the posterior penalty at each iteration. In fact, we must emphasize that as the data error misfit decreases, both the prior and posterior cost functional reduce to zero. Then, from expression (6.4) we note that when convergence is achieved, the nth forward model fits the data \( \mathbf{d} \). Thus, we may expect the the nth inverse solution to be a good approximation to the nonlinear EL equations while it provides an improved estimate of the measurement vector.

6.2. Experiment 2

In the second experiment, we assume errors in the forcing and the boundary conditions. In Fig. 7, we present the true and the inverse permeability fields for this case. The inverse permeability shows improvement in some parts of the domain. Fig. 8 shows the posterior variance for the parameter estimate computed from the expression (5.18) (with \( x = x' \)) at the final iteration. We note that at the bottom left of the domain the variance has not been reduced. For this experiment, convergence was achieved after four iterations. The time series for the nth forward solution, the true and the inverse solution at four measurement locations is presented in Fig. 9. We obtain a good fit to the measurements but the white noise present in the forcing of the true solution does not allow a better fit over the whole time interval. Fig. 10 shows the pressure profile at the measurement time \( t = 3T/4 \). Finally we present in Fig. 11 the pressure field at time \( T \) at which no measurements were taken. From this example it is concluded that the estimation of the permeability is overshadowed somewhat by the presence of other errors in the model. In addition, at the bottom left of the domain no measurement was taken. Then, the inverse model does not learn about a region where the forward model is quite different from the true solution.

Table 4 shows the information obtained at each iteration. Again, we observe convergence of the forward model
to the inverse estimate. While the inverse permeability does not appear to give as good a fit to the true permeability as in experiment 1, the $L^2$ error between the inverse and true permeabilities are almost identical to that obtained in experiment 1 (see Table 3).

6.3. Experiments 3 and 4

Suppose now that the only uncertainty in the model is the permeability. In experiment 3 the true solution is obtained as in experiment 2 but without errors in the forcing and the boundary conditions. It can be seen from Figs. 12 and 13 that the inverse permeability shows better improvement than experiment 2, where additional model errors were present. It is also shown that the posterior error covariance for the inverse has reduced compared to that in Fig. 8. Note that to obtain convergence requires more iterations than in experiment 2, but there is a greater reduction of the error in the permeability (final column of Table 5).
This example shows that even if no measurements are assimilated in a certain region of the domain, it is still possible to obtain good estimates as long as the forward model does not contain sources of errors that influence the estimation.

In the previous experiments we assumed that the true solution was obtained by adding pseudo-random errors to permeability, boundary conditions, forcing terms, etc. However, in experiment 4 we suppose that the true permeability is given by

\[ K(x, y) = \begin{cases} 
4 & \text{if } x \in [0, 1] \\
2 & \text{if } x \in (1, 2]. 
\end{cases} 
\] (6.5)

Fig. 14 shows the inverse permeability which improves significantly from the prior \( K = 3.0 \). With this experiment we observe that even if we do not have knowledge of the prior error statistics, it is still possible to obtain a reasonable parameter estimate.

From Table 6 we note again a reduction in the error between the inverse and the true permeability. However, at the final iteration \( n = 4 \) we observe a slight increase in that error. We remark once more that this information was presented as a way to understand the improvement of the inverse permeability over the prior. It should not be interpreted as a lack of convergence. What we have is simply that the inverse permeability that generates the inverse solution (at \( n = 4 \)) has slightly larger \( L^2 \) error than the previous inverse permeability (\( n = 3 \)). Nevertheless, the inverse solution (at \( n = 4 \)) is considerably better than the prior guess.

Table 5

<table>
<thead>
<tr>
<th>( n )</th>
<th>( | K^n - K^{n-1} |_{L^2(\Omega)} )</th>
<th>( \mathcal{J}^p )</th>
<th>( \mathcal{J}^n )</th>
<th>( | d - \mathcal{L}(p^n) |_2 )</th>
<th>( | p^n - p^f |_{L^2(\Omega)} )</th>
<th>( | K^n - K |_2 )</th>
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</table>

Experiment 3.
7. Conclusion

The numerical results of the previous section demonstrate that the representer method is potentially an efficient approach for finding a minimizer of the nonlinear inverse problem, arising in data assimilation for single-phase flow with poorly known permeability. Even with a small number of measurements, the estimated state variable (pressure) is close to the true solution at the measurement locations as well as in the entire domain. The algorithm also produces a parameter estimate (permeability) showing global improvement (in the \(L^2(X)\)-norm) with respect to the prior guess. Although it may be difficult to obtain, the user has to provide the source of error in the model. However, even if the error is distributed among different parameters (experiment 2) we can still expect to find improvement. Conversely, if the error is localized as for example in the permeability, we can obtain better global improvement (experiment 3) in the parameter and the state estimate.

The convergence of the algorithm presented in this paper does not imply convergence to the solution of the nonlinear EL equations. However, as can be seen from the numerical results, we are generating a sequence of forward models that converges to an inverse estimate that in turn satisfies a first order approximation to the nonlinear equations. The introduction of an extra representer for the parameter is an essential part in solving the linear state parameter estimation problem. This technique, applied previously by Valstar [10], was studied for the particular case of single-phase flow and transport and was shown to generalize the formulation of Bennett [4] for this model. We have proved that the representer method gives the solution to the linearized problem. The prior error covariances are essential to any theoretical result [7] since they actually smooth the parameter and therefore the solution. When regular prior error covariances are considered (Gaussians), good estimates of a discontinuous permeability (experiment 4) can be obtained with these techniques. Furthermore, the representer method provides expressions for estimating posterior error covariances that may be useful in subsequent work for testing the hypothesis assumed for the prior error statistics.

7.4 Experiment 4

The numerical results of the previous section demonstrate that the representer method is potentially an efficient approach for finding a minimizer of the nonlinear inverse problem, arising in data assimilation for single-phase flow with poorly known permeability. Even with a small number of measurements, the estimated state variable (pressure) is close to the true solution at the measurement locations as well as in the entire domain. The algorithm also produces a parameter estimate (permeability) showing global improvement (in the \(L^2(X)\)-norm) with respect to the prior guess. Although it may be difficult to obtain, the user has to provide the source of error in the model. However, even if the error is distributed among different parameters (experiment 2) we can still expect to find improvement. Conversely, if the error can be localized as for example in the permeability, we can obtain better global improvement (experiment 3) in the parameter and the state estimate.

The introduction of an extra representer for the parameter is an essential part in solving the linear state parameter estimation problem. This technique, applied previously by Valstar [10], was studied for the particular case of single-phase flow and transport and was shown to generalize the formulation of Bennett [4] for this model. We have proved that the representer method gives the solution to the linearized problem. The prior error covariances are essential to any theoretical result [7] since they actually smooth the parameter and therefore the solution. When regular prior error covariances are considered (Gaussians), good estimates of a discontinuous permeability (experiment 4) can be obtained with these techniques. Furthermore, the representer method provides expressions for estimating posterior error covariances that may be useful in subsequent work for testing the hypothesis assumed for the prior error statistics.

Acknowledgement

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Appendix A. Derivation of the parameter posterior error covariance

In Section 4, we derived an iterative algorithm that approximates the nonlinear generalized inverse problem of Section 3. Starting with a prior guess we iteratively com-

| Experiment 4. | ![Experiment 4](image) | Fig. 14. Left: true permeability field. Right: inverse permeability. |
pute an estimate \( (p^n, \lambda^n, K^n) \) that solves a linear inverse problem at the \( n \)th step for the penalty functional given by (3.21). This problem was stated as to find \( f^n, \beta^n, b_N^n, b_D^n \) and \( K^n \) in (3.20) such that \( p^n \) is a best fit in the least-squares sense given by \( J^n \). On the other hand, in Section 2 the error functions \( f^n, \beta^n, b_N^n, b_D^n \) and \( K^n \) were introduced in order to account for the uncertainty of the problem. Therefore, those error functions can be viewed as random fields with some properties. Assuming as before that the error covariances are given

\[
E(f^n(x,t), f^n(x', t')) = C_F(x, t, x', t'),
\]
\[
E(\beta^n(x,t), \beta^n(x', t')) = C_{\beta}(x, t, x', t'),
\]
\[
E(b_N^n(x,t), b_N^n(x', t')) = C_N(x, t, x', t'),
\]
\[
E(b_D^n(x,t), b_D^n(x', t')) = C_D(x, t, x', t'),
\]
\[
E(k^n(x), k^n(x')) = C_K(x, x'),
\]
\[
E(\epsilon_j, \epsilon_m) = W^{-1}_{jm}
\]
and uncorrelated ([4, Chapter 5])

\[
E(f^n, \beta^n) = 0, \quad E(\beta^n, b_N^n) = 0, \quad E(\beta^n, b_D^n) = 0, \quad E(\beta^n, k^n) = 0,
\]
\[
E(f^n, \epsilon_m) = 0, \quad E(\beta^n, \epsilon_m) = 0, \quad E(\epsilon_m, \epsilon_m) = \epsilon_m
\]
\[
E(f^n, \epsilon_m) = 0, \quad E(\beta^n, \epsilon_m) = 0, \quad E(\epsilon_m, \epsilon_m) = \epsilon_m
\]
\[
E(f^n, \epsilon_m) = 0, \quad E(\beta^n, \epsilon_m) = 0, \quad E(\epsilon_m, \epsilon_m) = \epsilon_m
\]

(A.1)

(A.2)

Note that during the iterative algorithm we assume the prior error covariances remain the same. In this section, we want to obtain a formula for the posterior error covariance for the parameter. In other words, we find the covariance for the error between the true and the inverse estimate of the parameter. Let \( (p^n, K^n) \) be the true solution of the \( n \)th problem which we assume is the solution of (3.20) for a set of error functions \( f^n, \beta^n, b_N^n, b_D^n \) and \( K^n \). Then, by (2.6) note that for each \( m = 1, \ldots, M \),

\[
E(d_m - \mathcal{L}_m(p^n), d_j - \mathcal{L}_j(p^n))
\]
\[
= E(\mathcal{L}_m(p^n) - p^n, \mathcal{L}_j(p^n) - p^n + \epsilon_j)
\]
\[
= E(\mathcal{L}_m(p^n) - p^n, \mathcal{L}_j(p^n) - p^n) + E(\mathcal{L}_m(p^n) - p^n, \epsilon_j)
\]
\[
+ E(\epsilon_m, \mathcal{L}_j(p^n) - p^n) + E(\epsilon_m, \epsilon_j).
\]

(A.3)

From the definition of the inner product in terms of the bilinear form (4.10), the operator defined in (4.9) and the definition of formal inverse (2.12), we compute

\[
\mathcal{L}_m(p^n - p^n) = (p^n - p^n, K^n - K^n - 1, \mathcal{R}_m) = E(\mathcal{L}_m(p^n) - \mathcal{L}_m(p^n), \mathcal{L}_j(p^n) - \mathcal{L}_j(p^n))
\]
\[
+ E(\mathcal{L}_m(p^n) - \mathcal{L}_m(p^n), \epsilon_j) + E(\epsilon_m, \mathcal{L}_j(p^n) - p^n) + E(\epsilon_m, \epsilon_j).
\]

(A.4)

Note that we are including Dirichlet boundary conditions for which the operator \( A^n \) (4.9) has an extra component \( A^n_D(p, K) = p|_{\Gamma_0}^n \). From (A.1) and (A.2),

\[
E(\mathcal{L}_m(p^n - p^n), \mathcal{L}_m(p^n - p^n))
\]
\[
= \alpha_j^n \mathcal{L}_j \mathcal{R}_m + \alpha_j^n \mathcal{L}_j \mathcal{R}_m + \alpha_j^n \mathcal{L}_j \mathcal{R}_m + \alpha_j^n \mathcal{L}_j \mathcal{R}_m
\]
\[
+ \alpha_j^n \mathcal{L}_j \mathcal{R}_m + \alpha_j^n \mathcal{L}_j \mathcal{R}_m + \alpha_j^n \mathcal{L}_j \mathcal{R}_m + \alpha_j^n \mathcal{L}_j \mathcal{R}_m
\]
\[
+ \alpha_j^n \mathcal{L}_j \mathcal{R}_m + \alpha_j^n \mathcal{L}_j \mathcal{R}_m + \alpha_j^n \mathcal{L}_j \mathcal{R}_m + \alpha_j^n \mathcal{L}_j \mathcal{R}_m
\]

(A.5)

while

\[
E(\mathcal{L}_m(p^n - p^n), \epsilon_j) = E(\epsilon_m, \mathcal{L}_j(p^n - p^n)) = 0.
\]

(A.6)

Again, from (4.9), (4.10) and (2.12) we obtain

\[
((r_m^n, y_m^n), (r_m^n, y_m^n)) = E(r_m^n, r_m^n, (r_m^n, y_m^n)
\]
\[
= \alpha_j^n \mathcal{L}_j \mathcal{R}_m + \alpha_j^n \mathcal{L}_j \mathcal{R}_m + \alpha_j^n \mathcal{L}_j \mathcal{R}_m + \alpha_j^n \mathcal{L}_j \mathcal{R}_m
\]
\[
+ \alpha_j^n \mathcal{L}_j \mathcal{R}_m + \alpha_j^n \mathcal{L}_j \mathcal{R}_m + \alpha_j^n \mathcal{L}_j \mathcal{R}_m + \alpha_j^n \mathcal{L}_j \mathcal{R}_m
\]
\[
+ \alpha_j^n \mathcal{L}_j \mathcal{R}_m + \alpha_j^n \mathcal{L}_j \mathcal{R}_m + \alpha_j^n \mathcal{L}_j \mathcal{R}_m + \alpha_j^n \mathcal{L}_j \mathcal{R}_m
\]

(A.7)

Comparing (A.5) and (A.7) we realize

\[
E(\mathcal{L}_m(p^n - p^n), d_j - \mathcal{L}_j(p^n)) = (r_m^n, y_m^n) = R_{m}^n + W_{m}^{-1}
\]

(A.8)

where the last equality comes from Remarks 1 and 2 as well as the definition of the representer matrix \( R^n \) which is clearly symmetric. Combining (A.3), (A.6), (A.7) and (A.1) we have

\[
E(d_m - \mathcal{L}_m(p^n), d_j - \mathcal{L}_j(p^n)) = R_{m}^n + W_{m}^{-1}
\]

(A.9)

Observation 1. Eq. (A.9) implies that \( R^n + W^{-1} \) equals the cross-covariance of the linearized model measurement misfit.

Observation 2. For each \( m = 1, \ldots, M \), the representers \( (r_m^n, y_m^n) \) are the cross-covariance between the error parameter and the \( m \)th measurement error.

Proof. From (2.6) and (A.2),

\[
E(k^n, d_m - \mathcal{L}_m(p^n)) = E(k^n, \mathcal{L}_m(p^n - p^n)) + E(\epsilon_m) = E(k^n, \mathcal{L}_m(p^n - p^n)) + E(\epsilon_m)
\]
\[
= E(k^n, \mathcal{L}_m(p^n - p^n)) = E(k^n, \mathcal{L}_m(p^n - p^n))
\]

(A.10)

Eq. (A.4) and the covariances relations (A.1) and (A.2) give us

\[
E(k^n, \mathcal{L}_m(p - p^n)) = E(k^n, f^n) + E(k^n, \beta^n) + E(k^n, b_N^n) + E(k^n, b_D^n) + E(k^n, K^n - K^n - 1) + E(k^n, \mathcal{R}_m) + E(k^n, \mathcal{R}_m)
\]
\[
= C_K \mathcal{R}_m = C_K \mathcal{R}_m = C_K \mathcal{R}_m = C_K \mathcal{R}_m = C_K \mathcal{R}_m = C_K \mathcal{R}_m = C_K \mathcal{R}_m = C_K \mathcal{R}_m
\]

(A.11)

Therefore,

\[
E(k^n(x), (d_m - \mathcal{L}_m(p^n)) = y_m^n(x).
\]

(A.12)
Now we derive the formula for the posterior error covariance for the parameter. Observe that

\[ E(K^n_T - K^n) = E\left(K^n_T - K^{n-1} - \sum_{i=1}^{m} \beta_i^{n,m} K^n_T - K^{n-1} - \sum_{i=1}^{m} \beta_i^{n,m}\right) \]

\[ = E(k^n, k^n) = 2E\left(k^n, \sum_{i=1}^{m} \beta_i^{n,m}\right) + E\left(\sum_{i=1}^{m} \beta_i^{n,m}, \sum_{i=1}^{m} \beta_i^{n,m}\right). \]

(A.13)

where we have used the fact that \( K^n_T = K^{n-1} + k^n \). We now define \( \gamma^n = (\gamma^n_1, \ldots, \gamma^n_M) \). From (5.17), (A.11) and the fact that \( R^n \) and \( W \) are symmetric,

\[ E(k^n(x), (\beta^n)^T \gamma^n(x')) = E(k^n(x), (d - \varphi(p^n_T))^T (R^n + W)^{-1} \gamma^n(x')) \]

\[ = E(k^n(x), (d - \varphi(p^n_T))^T (R^n + W)^{-1} \gamma^n(x')) \]

\[ = \gamma^n(x)(R^n + W)^{-1} \gamma^n(x'). \]

(A.14)

From (A.9)

\[ E((\beta^n)^T, (\beta^n)^T) = (R^n + W)^{-1} E((d - \varphi(p^n_T))^T (d - \varphi(p^n_T))^T) (R^n + W)^{-1} \]

\[ = (R^n + W)^{-1} (R^n + W)^{-1} \]

\[ = (R^n + W)^{-1}. \]

(A.15)

Thus,

\[ E((\beta^n)^T \gamma^n(x), (\beta^n)^T \gamma^n(x')) = \gamma^n(x) E(\beta^n, (\beta^n)^T) \gamma^n(x') \]

\[ = \gamma^n(x)(R^n + W)^{-1} \gamma^n(x'). \]

(A.16)

From (A.13), (A.14), (A.1) and (A.16) we finally obtain

\[ E(K^*_n(x) - K^n(x), K^*_n(x') - K^n(x')) = C_K(x, x') - \gamma^n(x)(R^n + W)^{-1} \gamma^n(x'). \]

(A.17)

References


