Shape Optimization Methods Locating Layer Interfaces in Geothermal Reservoirs

Simin Huang a*, Florian Wellmann a, Gabriele Marquart b, Michael Herty c, and Christoph Clauser b

a Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen University, Germany
b Institute for Applied Geophysics and Geothermal Energy, RWTH Aachen University, Germany
c Department of Mathematics, IGPM, RWTH Aachen University, Germany

Abstract

Subsurface structures have a strong influence on fluid flow and heat transport in geothermal systems. We examine whether the position and shape of an interface between two lithological bodies can be detected based on temperature-depth measurements. We use a level set function to describe the interface, and a shape optimization method in combination with the adjoint variable based on the heat transport equation to invert for position and shape. Specifically, we investigate how advective heat transport affects the identification of the interface and show that the method successfully retrieves interface positions in synthetic 2D cases of two-layer models.

Keywords: level set function; adjoint variable; shape optimization; inversion problem; geothermal reservoir; heat transport equation

1. Introduction

Inversion methods are widely applied to determine petrophysical properties, and increasingly also structural elements, of the subsurface. Oliver summarized in [1] the key developments in reservoir history matching including reparameterization of the model variables, computation of sensitivity coefficients, and uncertainty quantification.

* Corresponding author.
E-mail address: huang.simin@rwth-aachen.de
Associated issues and techniques of modeling uncertainty of Earth systems can also be found in [2]. We present here a shape optimization method with level set functions and adjoint variables to infer the position of subsurface geophysical layers, based on temperature data measured in boreholes. We study a synthetic 2D model with two layers of different petrophysical properties (i.e. thermal conductivity and permeability). The goal is to identify the interface position and shape from temperature depth data measured in several boreholes. This task is formulated as an optimization problem. A least-squares function is first established subject to the heat transfer equation governing the temperature field and its temporal variations. Instead of directly computing the gradient of the objective function, we compute the adjoint variable of temperature. A level set method is then used to represent the shape of the geological interface. The change of the level set function describes the evolution of the model during optimization iterations. The level set function follows a Hamilton-Jacobi equation and the zero level set is used to indicate location of the interface. With the adjoint variable and temperatures predicted from forward modeling of conductive and advective heat transport in the model, an artificial velocity is calculated at each grid point. This velocity is subsequently used for a stepwise update of the level set function and, therefore, the position of the layer. This procedure is repeated until a specified tolerance level is obtained and the position of the geological interface is retrieved.

In [3], Papadopoulos addressed the reconstruction of geophysical layers with the combination of the adjoint variable and the level set method for the case of heat conduction. We extended this work so that it can be used to compute adjoint variables for both conductive and advective heat transport cases. We describe the theoretical aspects of this extension in the next section, and then test our method in a synthetic case study in several model scenarios.

2. Methods

2.1. Forward Modeling

The forward problem is described by the heat transport equation for the fluid flow, which can be derived by considering the content of heat change of a control volume and applying Darcy’s Law and Gauss’ theorem [4]. The heat transport equation can be expressed as:

\[ \nabla (\lambda \nabla T - \rho_f c_f \nabla v) = \frac{\partial T}{\partial t} (\phi \rho_f c_f + (1 - \phi) \rho_m c_m) \] (1)

Where \( \rho_f \) is fluid density (kg m\(^{-3}\)), \( c_f \) is fluid specific heat capacity (J kg\(^{-1}\)K\(^{-1}\)), \( v \) is Darcy (filtration) velocity (m s\(^{-1}\)), \( \phi \) is porosity, \( \rho_f c_f \) is volumetric heat capacity of the fluid, \( \rho_m c_m \) is volumetric heat capacity of the rock matrix, \( \lambda \) is effective thermal conductivity of the saturated porous medium (W m\(^{-1}\)K\(^{-1}\)). Currently we only take the distribution of conductivity into consideration, assuming other parameters as constant. Also conductivity \( \lambda \) is assumed to be isotropic, so it is treated as a scalar.

2.2. Adjoint Method

In order to do shape optimization of the interface, the problem we are trying to solve here is to minimize the (quadratic) temperature residual under the constraint of the heat transport equation. To avoid directly computing the gradient of the objective function with respect to heat transport, we apply the adjoint method and compute the adjoint variable of temperature instead. Sirkes and Tziperman explained in [5] the process of continuous adjoint approach for deriving the adjoint equations, by considering a simple one dimensional advection-diffusion equation. For our case, similarly, we can first define an objective function:
\[ J = \frac{1}{2} \int_0^t \int_D \left( T_{\text{pre}} - T_{\text{obs}} \right) dx \, dt \] (2)

where \( T_{\text{pre}} \) is predicted temperature computed from forward modeling based on a predicted model and \( T_{\text{obs}} \) is observed temperature. The residual between predicted and observed temperature is integrated over a certain time \( t \) and region \( D \). Assume the objective function is minimized subject to a constraint function \( G \):

\[ G(T, \lambda) = 0 \] (3)

We identify equation (3) as the forward equation. Temperature \( T \) is the state variable, \( \lambda \) is the conductivity. By applying the method of Lagrangian multipliers [6] the adjoint equations are formed by adding the forward equation as constraints to the objective function and forming the Lagrangian function:

\[ L = J - \int_0^t \int_D \theta G(T, \lambda) \, dx \, dt \] (4)

where the Lagrangian multiplier \( \theta \) is the adjoint variable of temperature \( T \) and does not depend on \( \lambda \). When the derivative of \( L \) with respect to \( T \) equals to zero \( (\frac{\partial L}{\partial T} = 0) \), the Lagrangian function is at a stationary point, so that the objective function could be minimized \( (\frac{\partial J}{\partial T} = 0) \) subject to the constraint function \( G(T, \lambda) = 0 \).

\[ \frac{\partial L}{\partial T} = \frac{\partial J}{\partial T} + \frac{\partial}{\partial T} \left( \int_0^t \int_D \theta G(T, \lambda) \, dt \, dx \right) = 0 \] (5)

At such stationary point of \( L \), equation (5) is used for deriving the adjoint-state equation. By applying a Frechet derivative to \( L \) [3], from equation (5) we obtain:

\[ \nabla(\lambda \nabla \theta) + \rho c_f v \nabla \theta + \rho c_e \frac{\partial \theta}{\partial t} = \left( T_{\text{obs}} - T_{\text{pre}} \right) \] (6)

which is the adjoint-state equation. By solving this equation the adjoint variable \( \theta \) can be obtained. Because \( G(T, \lambda) = 0 \), from equation (4) we have:

\[ \frac{\partial J}{\partial \lambda} = \frac{\partial L}{\partial \lambda} \] (7)

By calculating the derivative of the Lagrangian \( L \) and introducing the velocity \( v_n = \mathbf{v} \cdot \mathbf{n} \) in the normal direction of the interface, a detailed derivation of \( dL(T, \lambda, \theta) \) using Hadamard formula for volume and surface integrals has been given in [3] as:
\begin{equation}
\quad dL = \int_{\partial \Omega} \int_{0}^{t} \left( \lambda_1 - \lambda_2 \right) \nabla \theta \nabla T \cdot \nabla \cdot \vec{n} \ d\Gamma \ dt + \epsilon \int_{\partial \Omega} \vec{v} \cdot \nabla \left[ \frac{\partial R}{\partial n} + kR \right] d\Gamma 
\end{equation}  

(8)

Where \( \partial \Omega \) is the interface we want to determine. The first term in equation (8), the multiplication of gradient of temperature, gradient of adjoint variable, normal velocity and difference between conductivity at the two layers is integrated over time \( t \) and along the interface. The second term in equation (8) is the regularization term, which will be explained in more detail below. Notice that \( \epsilon_n \) does not indicate that the geometry of the layers is actually changing. It is the velocity of points on the interface in the normal direction which we call artificial velocity and which changes during optimization iterations. In order for \( L \) to be positive, the velocity can be chosen as ([3], [7]):

\begin{equation}
\quad \epsilon_n = (\lambda_1 - \lambda_2) \nabla \theta \nabla T + \epsilon \kappa
\end{equation}  

(9)

where \( \epsilon \kappa \) is the multiplication of regularization parameter and local curvature.

2.3. Level Set Functions

Assume an open region \( \Omega \) is bounded by an interface \( \partial \Omega \) which moves under a certain velocity field \( \vec{v} \), to analyze the motion of the interface, Osher and Sethian [8] defined a smooth function \( \phi(t, x) \) to represent the interface which is chosen so that \( \phi(t, x) = 0 \). \( \phi \) is the level set function with such properties:  

\begin{align*}
\phi(t, x) &> 0 \quad \text{for} \quad x \in \Omega \\
\phi(t, x) &< 0 \quad \text{for} \quad x \in \Omega \\
\phi(t, x) &= 0 \quad \text{for} \quad x \in \partial \Omega
\end{align*}  

(10), (11), (12)

Let \( x \) be a point on the interface \( \partial \Omega \), by differentiating both sides of a level set function \( \phi(t, x) = 0 \) with respect to time we obtain a Hamilton-Jacobi-type equation:

\begin{equation}
\frac{\partial \phi(x, t)}{\partial t} + \frac{\partial x}{\partial t} \nabla \phi(x, t) = 0
\end{equation}  

(13)

Points on the interface are assumed to be moving only in the normal direction, as the motion in tangential direction does not change the shape [9] and the system is always well posed normal to the front [10]. Thus, only the normal component of the velocity field is needed and equation (13) can be rewritten as:

\begin{equation}
\frac{\partial \phi(x, t)}{\partial t} + \epsilon_n |\nabla \phi(x, t)| = 0
\end{equation}  

(14)

In our two-layer model, points on the interface are set to be zero, while points above and below the interface are initialized as signed distance function to the interface. In each iteration, points on the interface move in the normal direction with the velocity \( \epsilon_n \) for a certain length of time \( t \). The motion of the interface can then be captured by locating the zero level set.
2.4. Regularization

In order to compute stable optimization results with level set functions, regularization has to be used [8],[7]. A direct approach is to add a penalty term or a constraint to the minimization problem, which requires an appropriate regularization function $R$ and a regularization parameter $\varepsilon > 0$ ([9]). Then the objective function becomes:

$$ J = \frac{1}{2} \int_0^T \int_D \left( T_{pre} - T_{obs} \right) dx \, dt + \varepsilon \int_R d\Gamma $$

(15)

As explained in [3] and proved in [13], the shape derivative and shape gradient of the second term of the above equation can be given by:

$$ \varepsilon d\Omega \int_R d\Gamma = \varepsilon \int \frac{\partial R}{\partial n} + \kappa R d\Gamma $$

(16)

Where $\kappa$ is mean curvature of the interface. In our study we follow the work by Ito [11] and Papadopoulos [3] who chose the regularization functional as $R = 1$, such that we got the velocity expressed as equation (9). It has been suggested that adding a curvature term to the velocity provides regularization that works for tangentially smoothing of the interface ([10], [9], [8]). Chopp [12] also developed an algorithm for computing minimal surfaces by relating a surface to a given boundary and letting it move according to its mean curvature. By doing curvature regularization the level set function is modified as ([10])

$$ \frac{\partial \phi(x,t)}{\partial t} + \left( \frac{\nabla \phi(x,t)}{\nabla \phi(x,t)} - \nabla \phi(x,t) \right) \cdot \nabla \phi(x,t) = 0 $$

(17)

or equivalently:

$$ \frac{\partial \phi(x,t)}{\partial t} + (v_n + \varepsilon \kappa) \cdot \nabla \phi(x,t) = 0 $$

(18)

The mean curvature $\kappa = -\nabla \cdot \left( \frac{\nabla \phi(x,t)}{\nabla \phi(x,t)} \right)$ is calculated as ([9]):

$$ \kappa = \frac{2 \phi_x \phi_y \phi_z - \phi_y \phi_x^2 - \phi_z \phi_x^2}{(\phi_x^2 + \phi_z^2)^{3/2}} $$

(19)

Which allows computing the solution even when the interface is not a function.

3. Synthetic tests

The synthetic tests are performed on a 2D model area with width of 2.5 km and depth of 1.5 km. Temperature is set to 11 °C at the top boundary as a Dirichlet boundary condition. For model 2 and model 3 that are advection-dominated, at the top boundary, the hydraulic head is defined as a linear function decreasing from 930 m at $x = 0$ to
900 m at x = 2.5 km. Synthetic temperature data is assumed to be obtained from two vertical boreholes located at 0.65 km and 1.85 km. Temperature is assumed to be obtained vertically at each 50 meters. For the starting model, the predicted interface is a horizontal line at the depth of 1 km, with conductivity and permeability $\lambda_1 = 3.8 \text{ W m}^{-1} \text{ K}^{-1}$, $k_1 = 1.2 \times 10^{-14} \text{ m}^2$ and $\lambda_2 = 3.6 \text{ W m}^{-1} \text{ K}^{-1}$, $k_2 = 1.2 \times 10^{-15} \text{ m}^2$ for the two layers. Temperature is computed with a finite difference approach implemented in the program SHEMAT-suite [4]. The program uses an II’ scheme combining upwind and central differencing schemes. It is second-order accurate in space, and unconditionally stable. For solving the Hamilton-Jacobi equation (18), a third-order Runge-Kutta scheme is used for the time integration, weighted essentially non-oscillating (WENO) scheme is used for spatial discretization. The numerical grid of our model consists of 100 (horizontal) x 60 (vertical) grid nodes. Currently the regularization parameter is chosen by carrying out several synthetic experiments, and is set as 0.05 for all the three test cases discussed below.

3.1. Numerical results

We present the results for three test models. Model 1 and model 2 have the same real interface, while model 1 is set to be pure conductive and model 2 is advection-dominated. We also test model 3, which has a different interface and is advection-dominated. Both model 2 and model 3 have approximately the system Peclet number of around 3. The directions of fluid flow are shown in Fig. 2 (b) and Fig. 3 (b). All the three test cases require about 50 iterations to finally converge from an initially assumed arbitrary interface position to the real interface. Because we compute the adjoint variable instead of the direct gradient of temperature with respect to conductivity at each location, this step is in terms of computational cost almost equivalent to one more forward run, thus the total computation can be completed in very reasonable computing time.

By comparing the adjoint variable and artificial velocity of model 1 (pure conductive) and model 2 (advection-dominated), we can see that during the initial iteration phase, values of the adjoint variable are different, but these differences diminish as the interface position is approached during the optimization phase. As shown in Fig.1(b), Fig. 2(i), Fig.3(i), generally the optimization results show a good match between the predicted and real interface, for both shape and locations. For model 3, the interface between the boreholes is better matched than the remaining part, which indicates that the quality of the optimization results could be significantly affected by borehole locations and shape of the interface.

Other than these factors, the depth range and logging intervals of measured temperature data could also affect the quality of optimization results, which should also be taken into consideration. The results of model 2 are based on synthetic temperature data obtained vertically from boreholes at each 50 meters, we also tested the case with sparser temperature data availability at each 100 meters, which produce very similar optimization results, but require much more computing time (about 900 iterations to converge to the real interface compared to about 50 iterations) compared to the case of 50 m measurement intervals.

One additional numerical effect, which has to be taken into account, is the oscillation of the resulting layer close to the borehole positions. This effect can, for example, be observed in the optimisation results of model 2 in Fig. 2(i): at the 20th iteration, the identified layer has not yet converged to the true layer, and the layer is therefore moved upwards in the next iteration steps. However, at the 30th iteration, the layer position is now located above the true layer at locations around the boreholes. In the next iteration step, this behaviour results in a downward movement of the layer, and potentially a position below the true position, again. Following steps could result in more oscillations of this type, due to continuous overshooting around the expected layer position. This effect is mostly prominent in the area around the boreholes as the artificial velocity generally decreases with distance to the boreholes. Generally, applying regularisation can reduce these oscillation effects. However, proper regularization requires the estimation of a reasonable regularization parameter. A large regularization parameter is able to provide smooth interfaces, but may cause inaccuracy in the results. Currently we use experimentally derived values, which lead to a reasonable reduction in oscillation effects (0.05 in all three test models).
Fig. 1. (a) Model 1, the pure conductive case. (b) Optimization result for (i.e. estimated interface position) at the 1st, 10th, 20th, 30th, and the final iteration for model 1. (c) Adjoint variable at the 1st iterations for model 1. (d) Artificial velocity at the 1st iterations for model 1. (e) Adjoint variable at the 10th iterations for model 1. (f) Artificial velocity at the 10th iterations for model 1. (g) Adjoint variable at the 30th iterations for model 1. (h) Artificial velocity at the 30th iterations for model 1.
Fig. 2. (a) Model 2, the advection-dominated case. (b) Darcy velocity field for model 2. (c) Adjoint variable at the 1st iterations for model 2. (d) Artificial velocity at the 1st iterations for model 2. (e) Adjoint variable at the 10th iterations for model 2. (f) Artificial velocity at the 10th iterations for model 2. (g) Adjoint variable at the 30th iterations for model 2. (h) Artificial velocity at the 30th iterations for model 2. (i) Optimization result for (i.e. estimated interface position) at the 1st, 10th, 20th, 30th, and the final iteration.
Fig. 3. (a) Model 3, the advection-dominated case. (b) Darcy velocity filed for model 3. (c) Adjoint variable at the 1st iterations for model 3. (d) Artificial velocity at the 1st iterations for model 3. (e) Adjoint variable at the 10th iterations for model 3. (f) Artificial velocity at the 10th iterations for model 3. (g) Adjoint variable at the 30th iterations for model 3. (h) Artificial velocity at the 30th iterations for model 3. (i) Optimization result for (i.e. estimated interface position) at the 1st, 10th, 20th, 30th, and the final iteration for model 3.
4. Conclusions

The results of our synthetic case study indicate that our method can successfully reconstruct the position of a geological interface on the basis of temperature measurements from vertical boreholes in a hydrothermal flow field. We derived the theoretical concepts in detail. We first use the adjoint variable of temperature to obtain sensitivity estimates in the entire model domain at a very low additional computational cost. This implementation allows us to determine an artificial velocity of the level set function, which is used to describe the position of the layer interface. We show that this implementation allows us to efficiently retrieve the position of a layer between two geological units with distinctively different petrophysical parameters for the case of advective heat transport in geothermal systems. The results show that although the interface position and shape can be reconstructed with this method, its accuracy also significantly depends on a suitable choice of borehole locations. Therefore, one of the next research steps will be to determine the relationship between the (expected) shape of an interface and the borehole locations. After the problems mentioned above are solved, we may start to consider applying this method to multi-layer cases, and full 3D studies with real reservoir data.

References