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Accelerating Calibration of Natural State Geothermal Models

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ABSTRACT

Matching the pre-exploitation or natural state of a geothermal field is often problematic. The natural state is approximated by a steady state, achieved by running a geothermal model forward in time until the system is unchanging. The final simulation time may have to be many millions of years to achieve the goal, and therefore, steady state geothermal model simulations are regularly time-consuming. Furthermore, geothermal steady state models are prone to convergence problems with a steady state not being achieved. These issues may cause the inverse modeling process of matching model results to natural state data to be very time-consuming.

We propose a new methodology to aid derivative based inversion of natural state geothermal reservoir models. Model derivatives or sensitivities can be found by running the steady state simulation once and subsequently solving a system of linear equations with the number of right-hand sides determined by either N_m adjustable model parameters or N_d field observations of interest. By contrast, the standard approach for finding model sensitivities is by using finite differencing which requires solving at least N_m+1 nonlinear steady state simulations, each possibly requiring many time-steps. At each time-step the Newton-Raphson solution of the nonlinear equations requires the solution of at least one linear matrix equation making the forward simulations and therefore the inversion computationally intensive. The paper compares these approaches for synthetic steady state inversion problems, using TOUGH2 as the forward simulator. The results show the new methods to be superior to finite differencing in terms of computational time and resources.

1. INTRODUCTION

As a tool for understanding geothermal reservoir behavior, numerical modeling is limited by the ease of calibrating models to adequately match field observations. Advances in automatic inversion have made model calibration more viable. Increasingly automated calibration utilities such as PEST (Doherty, 2010) and iTOUGH2 (Finsterle, 2007) are being used to find suitable model parameters for geothermal reservoir models (e.g., Austria & O'Sullivan, 2015; Gunnarsson *et al.*, 2011; Kiryukhin & Miroshnik, 2012; Moon *et al*., 2014; Tateishi *et al.*, 2015).

One of the main barriers to geothermal model inversion is the number of time-consuming reservoir simulations needed for calibration of highly parameterized models. For both iTOUGH2 and PEST the main bottleneck is finding the sensitivities of model outputs to changes in the model parameters. Currently the sensitivities are found by perturbing parameters and using finite differences to approximate derivatives. Though flexible, this finite difference approach scales badly as the number of model parameters is increased, since the number of numerical simulations needed is proportional to the number of adjustable model parameters. The research described here aims to reduce the cost of model inversion by evaluating model sensitivities more efficiently by analytical means.

This paper demonstrates for natural state modeling of geothermal systems that considerable computational savings can be made by using an analytical approach to calculating sensitivity values. In the standard finite difference approach for calculating sensitivities many steady state problems must be solved, each involving a possibly lengthy transient approach to the steady state and at each time-step of the transient problem a large system of nonlinear equations must be solved. The analytic evaluation of sensitivities described here requires only one steady state problem to be solved followed by the solution of a system of linear equations with multiple right-hand sides. Thus there is the potential for considerable computational savings.

Though the focus here is on the stand-alone natural state modeling problem, the general approach can also be applied to automatic history matching of production data, or combined natural state and history matching (Bjarkason *et al*., 2015; Medina & Carrera, 2003). The only previous use of analytic evaluation of sensitivities in the geothermal context was by Rama Rao & Mishra (1996) who applied the analytical adjoint method to a sensitivity study for the Yucca Mountain waste repository site using TOUGH2. They used the TOUGH2 air, water and heat equation of state module, EOS3, to investigate how long-time values of gas saturation and liquid flow for a particular element in the model depended on absolute permeability and some of the parameters in the van Genuchten relative permeability and capillarity formulae. Although Rama Rao & Mishra considered a steady state model it was a very different type of problem to the steady state model investigated for modeling the natural state of geothermal fields (O'Sullivan et al., 2001). The natural state temperature distribution in a high temperature, convective geothermal system is strongly dependent on the permeability structure and thus calibration (by manual methods or inverse modeling) can be expected to effectively constrain the potential permeability structure. The improvement of inverse modeling methods for this type of natural state problem, unique to geothermal reservoir modeling, is the topic considered here.

The analytic calculation of sensitivities for inverse modeling investigated in this paper has been used in scientific disciplines related to geothermal reservoir modeling, namely: subsurface hydrology (Neumann, 1980a, 1980b) and petroleum engineering (Anterion *et al.*,

1989; Chavent *et al.*, 1975; Li *et al.*, 2003; Oliver & Chen, 2011; Oliver *et al.*, 2008). In the petroleum sector the analytical approach is widely used to efficiently calculate derivatives of nonlinear model outputs when matching transient oil and gas production data (Gao & Reynolds, 2006; Gao *et al.*, 2006; Oliver & Chen, 2011; Oliver *et al.*, 2008), as well as for optimal management of production and injection wells (Brouwer & Jansen, 2004; Jansen *et al.*, 2008; Kourounis *et al.*, 2014; Sarma *et al.*, 2006). In hydrology the analytical approach has been used to match both steady state and history data (LaVenue & Pickens, 1992; Medina & Carrera, 2003; Neuman & Carrera, 1985; Sykes *et al.*, 1985). Unlike geothermal and petroleum simulations, forward equations solved for a hydrological flow problem are often linear in the unknowns at every time-step and the steady state flow equations may also be relatively simple linear equations (Medina & Carrera, 2003).

The geothermal natural state problem is unique among subsurface flow problems because of its strong nonlinearity, requiring time-consuming forward simulations of a transient approach to the steady state. The high nonlinearity makes the analytical approach very attractive for natural state modeling of geothermal fields as only one, rather than many, forward steady state simulation is required.

2. STEADY STATE SIMULATIONS

The geothermal reservoir simulator used in this study is TOUGH2 (Pruess *et al*., 1999), which solves transient discretized mass and energy conservation equations. The equations solved by TOUGH2 at a given time-step for every finite volume can be compactly represented by the following residual vector $\boldsymbol{f}^k$ (Bjarkason *et al*., 2015)

$$\boldsymbol{f}^k\left(\boldsymbol{u}^k,\boldsymbol{u}^{k-1},\boldsymbol{m}\right)=\frac{1}{\Delta t^k}\left[\boldsymbol{M}\left(\boldsymbol{u}^k,\boldsymbol{m}\right)-\boldsymbol{M}\left(\boldsymbol{u}^{k-1},\boldsymbol{m}\right)\right]+\boldsymbol{FS}\left(\boldsymbol{u}^k,\boldsymbol{m}\right)=0 \tag{1}$$

Here the superscript k denotes values at the kth time-step, Δt^k is the time-step, $\boldsymbol{u}$ are the primary variables (block pressure, and temperature or saturation), $\boldsymbol{m}$ is a vector of the adjustable model parameters, $\boldsymbol{M}$ represents the mass and energy accumulation terms, and $\boldsymbol{FS}$ represents the inter-block fluxes and source terms (production or injection of mass or heat).

The nonlinear forward equations (1) are solved iteratively using Newton's method. Letting the superscript p denote values at the pth Newton iteration then the primary variables are updated according to

$$\boldsymbol{A}^{k,p-1}\left(\boldsymbol{u}^{k,p}-\boldsymbol{u}^{k,p-1}\right)=-\boldsymbol{f}^k\left(\boldsymbol{u}^{k,p-1},\boldsymbol{u}^{k-1},\boldsymbol{m}\right) \tag{2}$$

where

$$\boldsymbol{A}^{k,p-1}=\left[\frac{\partial \boldsymbol{f}^k}{\partial \boldsymbol{u}^k}\right]^{p-1} \tag{3}$$

is the forward Jacobian matrix.

For the natural state problem we are interested in the state where the reservoir is at equilibrium, established over a very long time and prior to production. This can be achieved by solving a steady state problem. Setting the accumulation part of equation (1) to zero the steady state problem is to find the state variables $\boldsymbol{u}_{st}$ for which the mass and energy fluxes balance out:

$$\boldsymbol{f}_{st}=\boldsymbol{FS}\left(\boldsymbol{u}_{st},\boldsymbol{m}\right)=0 \tag{4}$$

Solving the highly nonlinear steady state equations (4) directly is very difficult given an arbitrary initial guess for $\boldsymbol{u}_{st}$. For this reason the steady state problem is solved using a transient approach by solving (1) for a sequence of increasing time-steps. After a long enough simulation time and a large enough time-step Δt^k, the accumulation part of equation (1) becomes negligible and an approximate steady state has been reached.

The highly nonlinear behavior of the flow equations solved by TOUGH2 makes for long simulation times and as the time-step size increases convergence issues commonly arise (O'Sullivan *et al*., 2013, 2014). Convergence problems slow down the inversion process of matching pre-production data since it relies on running the TOUGH2 simulator many times. Each simulation of a state-of-the-art reservoir model may take many hours to complete. Our aim is to develop a method which reduces the number of nonlinear forward simulations and thus reduces the time spent calibrating a model.

3. MODEL INVERSION

To find model parameters $\boldsymbol{m}$ which respect the field observations $\boldsymbol{d}^*$ we try to minimize the objective function Φ defined by

$$\Phi\left(\boldsymbol{m}\right)=\left[\boldsymbol{d}\left(\boldsymbol{m}\right)-\boldsymbol{d}^*\right]^T\ \boldsymbol{C}_D^{-1}\left[\boldsymbol{d}\left(\boldsymbol{m}\right)-\boldsymbol{d}^*\right]+\beta\cdot R\left(\boldsymbol{m}\right) \tag{5}$$

Here $\boldsymbol{d}(\boldsymbol{m})$ are the model generated outputs from a TOUGH2 natural state simulation that are meant to match observations $\boldsymbol{d}^*$. We assume that all measurement errors are independent and Gaussian, giving a diagonal measurement covariance matrix $\boldsymbol{C}_D$ with observation error variances on its diagonal. We refer to the first term on the right-hand side as the observation mismatch. The final term,

$R(\boldsymbol{m})$, is a regularization term, which serves the mathematical purpose of creating a better conditioned inverse problem as well as making the model parameters honor prior ideas of their likely distribution and β (> 0) is a regularization factor.

There are various ways of solving the nonlinear minimization problem given by (5). The default approach of PEST and iTOUGH2 is to iteratively adjust $\boldsymbol{m}$ using variants of the Levenberg-Marquardt algorithm (Levenberg, 1944; Marquardt, 1963). These methods require the calculation of the so-called sensitivity matrix $\boldsymbol{S}$ (defined in equation (7)) at each iteration. The observation residual vector $\boldsymbol{r}$ is defined as

$$\boldsymbol{r}(\boldsymbol{m}) = \boldsymbol{d}(\boldsymbol{m}) - \boldsymbol{d}^* \tag{6}$$

If N_m is the number of adjustable model parameters $\boldsymbol{m}$ and N_d is the number of observations, then the elements of the N_d by N_m sensitivity matrix $\boldsymbol{S}$ are defined as

$$S_{ij} = \frac{\mathrm{d}r_i}{\mathrm{d}m_j} \tag{7}$$

Finding these derivatives efficiently and accurately is an important aspect of speeding up the Levenberg-Marquardt based inversion process. Inaccurate derivatives may corrupt the inversion process (Doherty, 2010).

3.1 Finite Differences

The current approach, used in PEST and iTOUGH2 for example, is to approximate the derivatives in (7) by finite differences, obtained by running multiple TOUGH2 simulations. The default method is the forward difference scheme, which has the lowest computational cost, but more accurate and computationally more expensive multi-point options can be used (see below and Doherty, 2010; Finsterle, 2007). Using parameter perturbations of size Δm_j and denoting the jth unit vector as $\boldsymbol{e}_j$, the finite forward difference scheme gives

$$S_{ij} = \frac{\mathrm{d}r_i}{\mathrm{d}m_j} \approx \frac{r_i\left(\boldsymbol{m} + \Delta m_j \boldsymbol{e}_j\right) - r_i\left(\boldsymbol{m}\right)}{\Delta m_j} \tag{8}$$

To calculate the full sensitivity matrix $\boldsymbol{S}$ this approach requires N_m+1 time-consuming nonlinear TOUGH2 simulations. Additionally, the derivatives found according to (8) have limited accuracy due to machine rounding and truncation errors. Higher order finite difference methods can be used to obtain more precise derivatives than those offered by first order forward differences. However, the improved accuracy comes at the cost of having to run even more nonlinear forward simulations. If greater accuracy is needed, both iTOUGH2 and PEST offer the option of evaluating the sensitivities using the two-point central difference scheme:

$$S_{ij} = \frac{\mathrm{d}r_i}{\mathrm{d}m_j} \approx \frac{r_i\left(\boldsymbol{m} + \Delta m_j \boldsymbol{e}_j\right) - r_i\left(\boldsymbol{m} - \Delta m_j \boldsymbol{e}_j\right)}{2\Delta m_j} \tag{9}$$

This necessitates two forward runs for each parameter to which the central scheme is applied. PEST also offers derivative stencils using more points, but those will not be discussed here because of their high computational cost.

The finite differencing approach has two main advantages. Firstly, it allows for great flexibility in the choice of parameters and simulation techniques, since the method only deals with the direct inputs and outputs of the simulation code. Secondly, each finite difference perturbation used to evaluate the sensitivity matrix can be solved independently and in parallel using separate processors. There are parallel versions of both iTOUGH2 (Finsterle, 2010) and PEST (Doherty, 2010; Hunt *et al.*, 2010) which exploit this aspect to speed up the inversion process.

3.2 Analytical Derivatives

For evaluation of accurate model sensitivities, analytical approaches offer an efficient means. Bjarkason *et al*. (2014, 2015) considered the benefits of using analytical ways of calculating sensitivities for transient TOUGH2 simulations for history matching of production data. It can be even more advantageous to apply those ideas to the natural state problem.

Differentiating the steady state equations (4) we find that the sensitivities of every primary variable at the steady state solution $\partial \boldsymbol{u}_{st}/\partial \boldsymbol{m}$ can be found by solving one linear system with N_m right-hand sides:

$$\boldsymbol{A}_{st}\left[\frac{\partial \boldsymbol{u}_{st}}{\partial \boldsymbol{m}}\right] = -\boldsymbol{G}_{st} \tag{10}$$

where

$$\boldsymbol{A}_{st} = \frac{\partial \boldsymbol{f}_{st}}{\partial \boldsymbol{u}_{st}} \;;\; \boldsymbol{G}_{st} = \frac{\partial \boldsymbol{f}_{st}}{\partial \boldsymbol{m}} \tag{11}$$

No extra computation is required to create $\boldsymbol{A}_{st}$, since it can be approximated by the flux and source part of the final forward Jacobian at the last time step of the natural state simulation. The $\boldsymbol{G}_{st}$ matrix is often simple to calculate because the governing equations (1) are linear in the common parameters that we wish to determine, i.e. permeabilities and mass flows of deep inputs. Under these circumstances the terms in $\boldsymbol{G}_{st}$ can be extracted with a little extra effort from the source terms and the inter-block fluxes that TOUGH2 has previously calculated (again at the last time step of the natural state simulation).

The sensitivity matrix is then found, after solving (10) for $\partial \boldsymbol{u}_{st}/\partial \boldsymbol{m}$, using

$$\boldsymbol{S} = \frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}\boldsymbol{m}} = \frac{\partial \boldsymbol{r}}{\partial \boldsymbol{m}} + \boldsymbol{C}_{st}\left[\frac{\partial \boldsymbol{u}_{st}}{\partial \boldsymbol{m}}\right] \tag{12}$$

where

$$\boldsymbol{C}_{st} = \frac{\partial \boldsymbol{r}}{\partial \boldsymbol{u}_{st}} \tag{13}$$

The matrix $\boldsymbol{C}_{st}$ is easy to evaluate for natural state observations, which are mostly downhole temperatures as well as reservoir pressures at sparse locations. Both the downhole temperatures and pressures are usually represented by simple linear combinations of block temperatures and pressures.

We shall refer to the above analytical approach as the direct method. This approach is in stark contrast to the finite difference one, for which we need to solve at least N_m natural state simulations in addition to the first unperturbed one. Let N_t denote the number of simulation time-steps needed to reach a steady state and N_{NR} be the average number of Newton-Raphson iterations for each time-step. It follows that the extra cost of forward differences is $N_t N_{NR} N_m$ linear solves. In terms of linear solves the added cost of the direct steady state method is therefore around $N_t N_{NR}$ times less than the cost of finite differencing.

If the number of model parameters N_m exceeds the number of steady state observations N_d, the adjoint method (Li *et al.*, 2003) should be considered. For the adjoint approach we solve for a matrix of Lagrange multipliers $\boldsymbol{\Psi}_{st}$:

$$\left[\boldsymbol{A}_{st}\right]^T \boldsymbol{\Psi}_{st} = -\left[\boldsymbol{C}_{st}\right]^T \tag{14}$$

Here (14) is a linear problem with N_d right-hand sides. Now the sensitivities are calculated using

$$\boldsymbol{S} = \frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}\boldsymbol{m}} = \frac{\partial \boldsymbol{r}}{\partial \boldsymbol{m}} + \left[\boldsymbol{\Psi}_{st}\right]^T \boldsymbol{G}_{st} \tag{15}$$

In either case, solving (10) or (14), savings can be made by using linear matrix tools suitable for multiple right-hand side problems. In our current work we have used the direct sparse solver SuperLU available within Python's SciPy library. Using the direct approach, time is saved since we only need to find an LU factorization of the relevant coefficient matrix once. The LU factors can then be shared for all right-hand sides. If this approach becomes too slow we may also consider block Krylov methods (Gutknecht, 2007), which are inexact methods designed to solve multiple right-hand sides. However, inexact Krylov methods rely heavily upon using a suitable pre-conditioner.

For a large sensitivity matrix (large N_d and N_m), forming the full sensitivity matrix $\boldsymbol{S}$ may be an overwhelming task. In that case methods which do not require explicit computation of $\boldsymbol{S}$ (e.g. truncated singular value decomposition to solve the Levenberg-Marquardt updates or using Quasi-Newton methods) can be applied efficiently using the analytical approach (Gao & Reynolds, 2006; Oliver *et al*, 2008; Tavakoli & Reynolds, 2010; Zhang & Reynolds, 2002). These are not considered here.

4. VERTICAL SLICE MODEL

The following results were found using a 3.40 GHz Intel i7-4770 CPU with 16 GB RAM. For our experiments we used AUTOUGH2, which is University of Auckland's version of TOUGH2 (Yeh *et al*., 2012), as our reservoir simulator. The AUTOUGH2 code was edited and recompiled to write out the necessary information needed for the adjoint and direct methods. The new outputs are written in HDF5 binary format, for efficiency and numerical precision. This new compiled code was used for all forward simulations while running PEST with the sensitivities evaluated using either the direct method or the adjoint method. When running PEST inversions using finite differencing the forward simulations used the normal AUTOUGH2 code without the HDF5 output format. AUTOUGH2 input and output files were read, run and edited using PyTOUGH (Croucher, 2011, 2014; Wellmann *et al.*, 2012). The analytical derivative methods were implemented using Python code.

Here is a summary of how PEST was run using the analytical approach:

1) PEST begins by running the forward problem for the initial parameter set and calculates the initial objective function.
2) The simulated observations and special HDF5 outputs are read from the first forward run.
3) The $\boldsymbol{A}_{st}$, $\boldsymbol{G}_{st}$ and $\boldsymbol{C}_{st}$ matrices are constructed from the natural state results (final time-step), and the sensitivity matrix is calculated using either the direct or adjoint method and written to output using PEST readable format.

4) Using the sensitivity matrix from the file, PEST attempts to find updated model parameters, which lower the objective function, based on the Levenberg-Marquardt approach. Every attempt to update the parameters requires a forward simulation.
5) PEST records the best model parameters found in step 4).
6) If one of the stopping criteria is met PEST exits with the best model parameters found to that point.
7) Otherwise find and read the special HDF5 outputs and simulated observations corresponding to the forward run using the best update to the model parameters.
8) Repeat step 3) and onwards.

To test the method we constructed a two-dimensional vertical slice model. For the simulations we used the pure water equation of state module EOS1. The model represents a rectangular vertical domain, 1,600 m deep and 2,000 m long in the horizontal direction, which consists of six rock types. The model structure is depicted in Figure 1. The numerical grid has 8,100 elements, 8,000 of which are cubes (20 m × 20 m × 20 m). The remaining 100 elements are large boundary blocks at the top of the model implementing constant pressure and temperature boundary conditions. The top boundary has a constant pressure of 1 atm and is at a constant temperature of 15°C. At the base of the model there is a constant heat flux of 80 mW/m^2, except at five blocks where there are inputs of very hot water. A total flow of 0.1 kg/s at an enthalpy 900 kJ/kg is spread over the five left-most blocks at the base of the model depicted in Figure 1. The side boundaries are closed. We used harmonic weighted absolute permeabilities at block interfaces (O'Sullivan *et al*., 2013) and apart from their permeabilities, all six rock types have the same parameters. Figure 2 shows the base ten logarithms of the absolute horizontal and vertical permeabilities of the true system. Here the units of all permeabilities are m^2. All rock types have a porosity of 10%, the rock grain density is 2,500 kg/m^3, a thermal conductivity of 2.5 W/(m·K) and a rock specific heat of 1.0 kJ/(kg·K). Of these four parameters only thermal conductivity affects the natural state results.

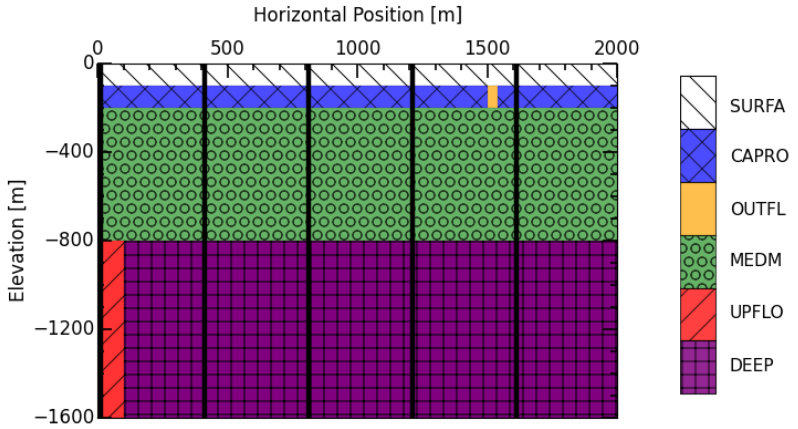

Figure 1: The true vertical slice model, showing the distribution of the six rock types. Locations of the five observation boreholes are indicated by the long vertical black lines.

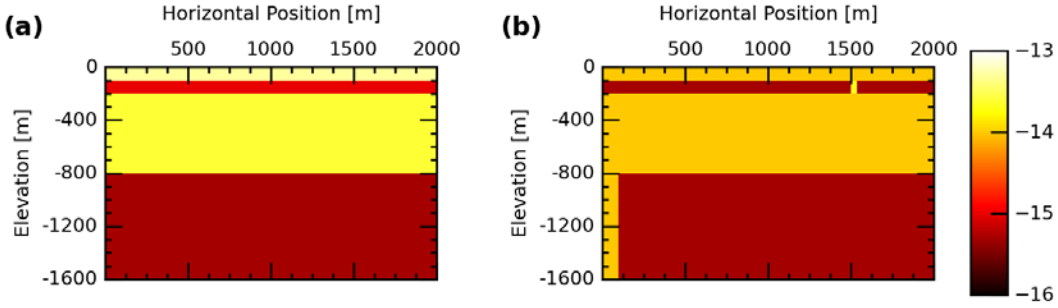

Figure 2: The true formation permeabilities: (a) logarithm of the horizontal permeability k_x; (b) logarithm of the vertical permeability k_z.

For the first simulation of an inversion the initial conditions were set to be homogeneous with all block pressures and temperatures equal to the top boundary conditions specified earlier. To accelerate subsequent natural state simulations the initial conditions were replaced at the beginning of each PEST iteration with the natural state conditions found using the most recently updated model parameters. This is especially helpful for the finite difference forward simulations, since small changes in model parameters are not likely to result in large changes in the final steady state primary variables.

For natural state conditions we ran simulations to a target time of 10^{16} s. All simulations were limited to a maximum of 500 time-steps, to make sure that computational times were always easily manageable. If the final target time was not reached by the maximum number

of time-steps, the assumption was made that the last time-step solution was a reasonable approximation to the steady state. However, for results presented here the maximum number of time-steps was never reached.

We created artificial natural state data by running the true model to steady state and selecting steady state temperatures down five vertical boreholes, see Figure 1. Observations were taken from every third model block intersected by each well, giving 135 temperature observations in total. Finally, random Gaussian noise with zero mean and a σ_d = 0.5°C standard deviation was added to the simulated temperatures to give the final observations used for the synthetic inversion study. The observations are shown in Figure 3.

PEST was used to invert the synthetic data. For the inversion process the observation noise level was assumed to be known, and then the measurement covariance matrix had all diagonal elements equal to the actual error variance σ_d^2. The standard approach of using finite differenced sensitivities was compared against results using analytically derived sensitivities. Two inversion problems were considered. For the first problem we assumed the rock structure was known and inverted for the horizontal and vertical permeabilities of the six rock types. In the second problem the rock structure was not assumed to be known. Instead the model was subdivided up into 320 patches of 5 × 5 blocks, each with its own rock type. Thus in this case the problem was to invert for the permeabilities of 320 rock types, giving a total of 640 adjustable parameters. In both cases all other model parameters were taken as known. For both inversion problems the initial guess of all log-transformed permeabilities was log(k) = -15. The adjustable log-permeabilities were limited to a maximum of -13 and a minimum of -16.

The natural state downhole temperatures given by the initial parameters are shown in Figure 3. The initial measurement misfit had a value of 2.4×10^6. For these tests we ran PEST in serial mode, though parallel versions of PEST should be considered when using finite differencing for large problems. Implications of using the parallel mode are discussed later in the section on the 640 parameter problem.

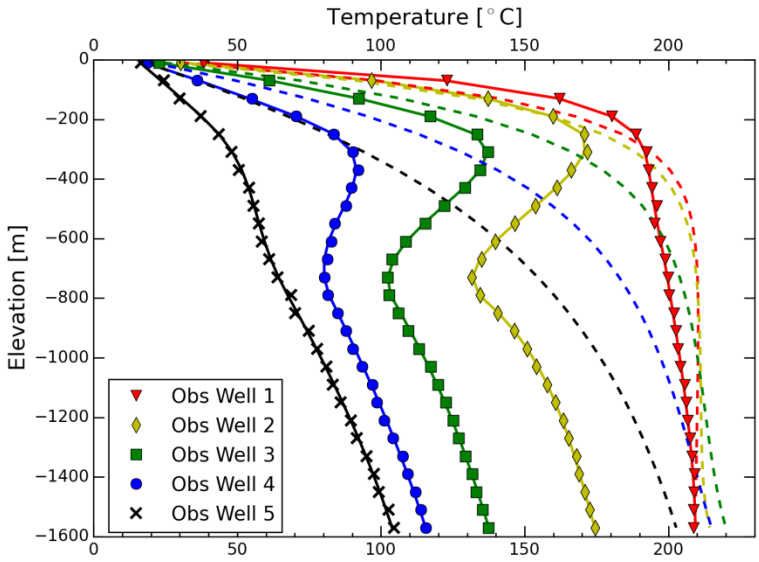

Figure 3: Observed downhole temperatures (markers), matched profiles (solid lines) and temperature profiles at commencement of the inversion (dashed lines). The wells are those shown in Figure 1, numbered from left to right.

4.1 Inversion of 6 Rock Types

As an initial test the horizontal and vertical permeabilities of the six rock types shown in Figure 1 were selected as unknowns. The formation structure, in terms of the extent of each rock type, was taken to be known. For this inversion problem the regularization term in equation (5) was chosen in terms of prior parameter information:

$$\beta \cdot R(\boldsymbol{m}) = \left[\boldsymbol{m} - \boldsymbol{m}_{\text{pr}}\right]^T \boldsymbol{C}_M^{-1} \left[\boldsymbol{m} - \boldsymbol{m}_{\text{pr}}\right] \tag{16}$$

Here $\boldsymbol{m}_{\text{pr}}$ is the prior estimation of the parameters, which was taken to be the initial guess for the model parameters at the start of the inversion. For our purposes the prior covariance matrix $\boldsymbol{C}_M$ was chosen to be a diagonal matrix with unit variances on the diagonal, approximately reflecting the distribution in the adjustable log-permeabilities. Adding priors to the inversion process should help deter changes in insensitive parameters, which could otherwise be unnecessarily shifted towards their upper or lower parameter bounds.

We inverted the synthetic data with PEST using forward differences, central differences and the direct method to evaluate the sensitivity matrix $\boldsymbol{S}$. The adjoint method was not tested for this problem because the number of observations is far greater than the number of adjustable parameters. The finite difference methods used 1% parameter perturbations for finding the model sensitivities. Results of the inversions using those three methods are shown in Table 1.

All the methods performed similarly with regard to the number of iterations needed to complete the inversion. All three methods concluded with approximately the same objective function, though the forward difference method terminated with a slightly higher

objective than the other methods. Note that the observation mismatch of the true model parameters is drawn from a chi-squared distribution with an expectation value of N_d (Doherty, 2015; Oliver *et al.*, 2008). Thus for the problem discussed here we expect for an inversion to obtain an observation mismatch of about N_d = 135. All three methods managed to obtain an observation mismatch below that expected value. The matched temperature profiles found using the direct method are shown in Figure 3. Results of the other inversions are nearly indistinguishable from the profiles shown in Figure 3.

Table 1: Inversion results using PEST for the 12 parameter natural state problem using forward differentiation (FWD), central differentiation (CNTRL) and the direct method.

Derivative Method	PEST Iterations	Nonlinear Simulations	Sensitivity Evaluations	Time [s]	Objective Function	Observation Mismatch	Prior Mismatch
FWD	28	421	28	3,670	131.47	125.61	5.86
CNTRL	26	703	26	5,930	131.33	125.70	5.63
Direct	28	82	28	866	131.33	125.67	5.67

The reason why the central and direct methods obtained a slightly lower objective function may be attributable to those two methods using more precise model derivatives. Further tests are needed though to make a definitive conclusion. For this test case the central difference scheme completed the inversion process in the fewest number of iterations. Nevertheless, the direct method followed quite a similar path to the central difference method. The direct method would have also finished after 26 iterations with the same objective function value had it not found a slightly lower objective function.

The main aspect we are interested in is the computational savings made using the analytical approach. Assuming we know the cost of running the analytical sensitivities, we can estimate the attainable relative speed up. If we define ε as the average ratio of the execution time needed for an analytical calculation of the sensitivity matrix to the time needed for one nonlinear forward simulation, then an estimate of the relative speed-up attained by using the analytical method over forward differentiation, at each optimization iteration, is

$$\eta = \left(N_m + N_\lambda\right) / \left(\varepsilon + N_\lambda\right) \tag{17}$$

Here N_λ is the average number of attempts at updating the objective function during a PEST iteration. The above equation assumes that N_λ is the same for both methods. Ideally, if the analytical derivative evaluations take an insignificant amount of time, the maximum speed up we can attain is

$$\eta = 1 + N_m / N_\lambda \tag{18}$$

For our runs using PEST the average number for N_λ is about three and thus the best we can expect from the analytical approach for 12 parameters is that it is 5 times faster than using finite differences. This is in agreement with the ratio of forward simulations used by the two methods which is 5.2. Comparing the computational times given in Table 1 the direct method was at least 4.2 times faster than forward differencing, indicating that the cost of evaluating the sensitivity matrix using the direct method was about half the cost of a nonlinear forward simulation. As we would expect the central difference scheme is about twice as slow as forward differencing.

Both iTOUGH2 (Finsterle, 2007) and PEST (Doherty, 2010) can be used to approximate the uncertainty of inverted parameters using a local sensitivity analysis. The local sensitivity analysis uses the sensitivity matrix of the inverted model parameters and an assumption of sufficiently linear observation residuals to quantify model parameter uncertainty. Table 2 shows, for the three inversion approaches, the estimated parameters and possible uncertainty bounds, found according to a linear sensitivity analysis with PEST. Apart from the estimated vertical permeability of the rock type SURFA, which is at the top of the model, all of the estimated permeabilities and their uncertainty intervals agree well with the true permeabilities. Understandably the permeabilities of the two largest formations MEDM and DEEP were estimated with the greatest precision. The vertical permeability for the rock type UPFL is well determined, probably because of its vertical extent and the fact it is the main conduit for the hot mass flow from the bottom. The evaluated permeabilities and their estimated uncertainties are generally in good agreement between the three methods.

4.2 Inversion of 320 Rock Types

To test the analytical sensitivity methods further we created a more demanding 640 parameter inversion problem. The model setup is the same as before, however, as discussed above we do not assume knowledge of the six rock types. Instead the model domain, less the boundary blocks, was divided up into 320 (5 × 5) patches, each with its own rock type. To identify such a large number of parameters we need to employ spatial smoothing through the regularization term. For a parameter m which varies as a function of space we can for instance choose to minimize the L2 norm of its gradient over the model domain of volume V:

$$R(m) = \int_V \nabla m \bullet \nabla m \, \mathrm{d}V \tag{19}$$

Table 2: Estimated horizontal (k_x) and vertical (k_z) permeabilities for the inversion of the 6 rock types using the forward difference (FWD), central difference (CNTRL) and direct methods. The indicated parameter uncertainties are 95% confidence intervals using linear sensitivity analysis. Sensitivity methods used for the analysis: *forward differences, †central differences and ‡direct method.

	SURFA		CAPRO		OUTFL		MEDM		DEEP		UPFL	
	-logk_x	-logk_z	-logk_x	-logk_z	-logk_x	-logk_z	-logk_x	-logk_z	-logk_x	-logk_z	-logk_x	-logk_z
True	13.30	14.00	15.00	15.30	15.00	13.70	13.60	14.00	15.30	15.30	15.30	14.00
FWD*	15±11	14.7±0.3	15.0±0.8	15.1±0.3	15±36	14±10	13.61±0.02	13.98±0.04	15.32±0.09	15.2±0.1	15±7	14.00±0.05
CNTRL†	15±11	14.7±0.4	14.9±0.8	15.1±0.3	15±36	14±8	13.61±0.02	13.98±0.04	15.32±0.09	15.2±0.1	15±7	14.00±0.04
Direct‡	15±11	14.7±0.4	15.0±0.8	15.1±0.2	15±38	14±7	13.61±0.02	13.98±0.04	15.32±0.09	15.2±0.1	15±7	14.00±0.04

The regularization term used here for the 640 parameter problem was

$$R(\boldsymbol{m}) = \sum_i \sum_j \left\{ \left[\log\left(k_x^i\right) - \log\left(k_x^j\right) \right]^2 + \left[\log\left(k_z^i\right) - \log\left(k_z^j\right) \right]^2 \right\} + \sum_i \left[\log\left(k_x^i\right) - \log\left(k_z^i\right) \right]^2 \tag{20}$$

The first term in the above equation is an approximation of (19) for the log-transformed permeability field; the summation is over all rock types i and their nearest neighbors j. The last term in (20) represents the fact that we expect similar values for the vertical and horizontal permeabilities. Note that we did not include a prior Tikhonov term as in equation (16). Because we did not have prior ideas for an optimal value of the regularization factor β, we allowed PEST to vary β throughout the inversion process. PEST changes the regularization weighting factor at the start of each iteration, using some linearity assumption and the sensitivity matrix (Doherty, 2010). Inversion was terminated by PEST when the observation mismatch had been reduced below N_d which is a reasonable target for the observation mismatch; low enough to show the effectiveness of our inverse scheme but likely to be high enough to avoid over-fitting.

Figure 4 compares sensitivity values found using the direct method with the two finite difference methods used in this work. The sensitivity values shown are for the initial guess of the inversion. As expected the central difference evaluated sensitivities were in better agreement with the analytical derivatives than those calculated with the forward difference method. Most of the values found using central differences were only about one-hundredth of a percent away from sensitivities derived using the direct method. The forward method on the other hand gave values which mostly deviated by about 1% away from the analytically evaluated sensitivities. The adjoint method was found to agree with the direct method, mostly within a ten-thousandth of a percent and all within a percent.

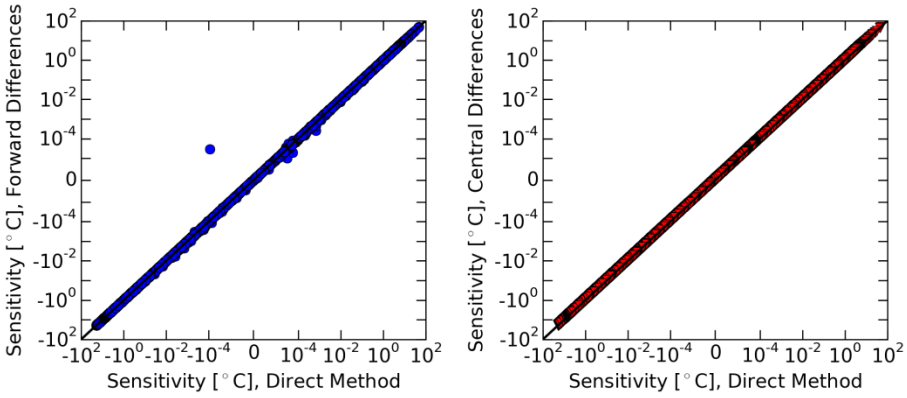

Figure 4: Comparison of sensitivity values for the 320 rock type natural state problem. The black diagonal lines are for the case of perfect agreement.

The results of inverting for the 640 permeability values are shown in Table 3. The central difference method was not tested since the forward difference method already took about a day to converge and the central method would have taken about twice as long. For this problem the adjoint method was also tested since the number of observations was about a fifth of the number of parameters. In terms of the number of iterations and objective function values all three methods performed similarly, but the finite difference method required an extra iteration. The main result is that the analytical methods were over a hundred times faster than the finite difference approach. Thus the analytical methodology was a definite success. The adjoint method was slightly faster than the direct method since for this problem there are fewer right-hand sides in equation (14) than in equation (10).

Table 3: Inversion results using PEST for the 640 parameter natural state problem using forward differentiation (FWD), the direct method and the adjoint method.

Derivative Method	PEST Iterations	Nonlinear Simulations	Sensitivity Evaluations	Time [s]	Objective Function	Observation Mismatch	$R(\boldsymbol{m})$	β
FWD	17	10,950	17	80,000	492.35	134.53	53.88	6.64
Direct	16	49	16	725	489.14	134.69	53.76	6.59
Adjoint	16	49	16	673	489.12	134.69	53.76	6.59

The evaluated permeability distributions for the 320 rock types are shown in Figure 5. All three inversions are nearly identical. These results can be compared with the true permeabilities shown in Figure 2. The results display the main features of the actual system, i.e., a large low permeability structure at depth, a high permeability structure across the system at a medium depth and the high vertical permeability is clearly seen in the upflow zone. The caprock and surface permeabilities are badly resolved. These results are in line with the results given Table 2 for the structurally correct 12 parameter problem.

From Table 3 we can estimate the relative speed-up per iteration when using either the direct or adjoint methods. Taking the ratio of the time spent for each iteration using forward differences over the time used by the analytical methods we find that

$$\eta \approx 110 \tag{21}$$

This indicates that for the 640 parameter problem the added cost of the analytical approach is only about three natural state simulations, $\varepsilon \approx 3$. This is only about six times the cost of finding the sensitivity matrix for the 12 parameter problem. According to equation (18) the maximum serial speed-up we could have attained using PEST would have been $\eta = 214$, for $N_\lambda = 3$. The improvement we made is not far off this maximum value.

To achieve this type of result using finite differencing we would need a considerable number of parallel processors run in unison by PEST. For enough processors the N_λ attempted updates can be run in parallel at a cost of the order of one simulation run. The main cost will be N_m forward simulations needed to construct the sensitivity matrix. Running the finite difference approach using parallel processors we would need access to approximately N_{pr} (given by (22)) CPUs to be as fast as using the serial steady state analytical approach.

$$N_{\mathrm{pr}} \approx N_m / \left(\varepsilon + N_\lambda - 1\right) \tag{22}$$

Therefore, for this 640 parameter problem we would have needed about 130 CPUs to obtain computational speed comparable to that found using the analytical methods. The analytical approach can therefore offer timely inversions using a lot less hardware.

Concerning the analytical approach and parallelization, there are a few options. As discussed earlier the N_λ trial updates at each inversion iteration can be run in parallel. Another option would be to use parallel algorithms to solve the forward problems (2) in parallel. Similarly, the linear direct and adjoint equations can be solved using parallel linear equation solvers. However, the parallel efficiency may be low for this approach. In our opinion those with access to large CPU clusters can best utilize parallelization by use of the analytical approach for advanced uncertainty quantification. Using an approximate Markov chain Monte Carlo approach, multiple model realizations and/or conceptual models can be inverted efficiently in parallel using an approach called Randomized Maximum Likelihood (Oliver *et al.*, 2008; Oliver *et al.*, 1996) to give an approximate probability distribution of the model parameters. This would achieve high parallel efficiency because communication with each CPU is only needed at the start and finish of distinct inversions.

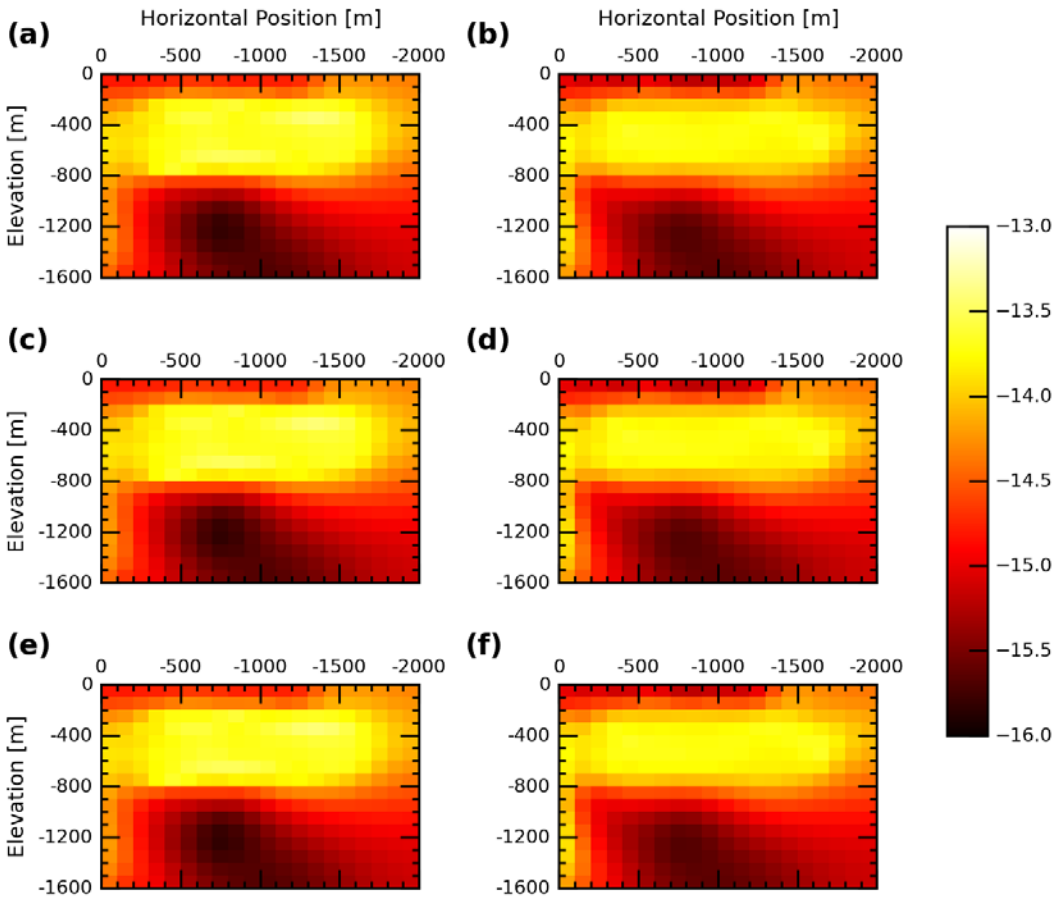

Figure 5: Estimated log-transformed permeabilities of 320 rock types using PEST: (a) horizontal and (b) vertical permeabilities found using forward finite differences; (c) horizontal and (d) vertical permeabilities results from the direct method; (e) horizontal and (f) vertical permeabilities according to the adjoint method.

5. FUTURE WORK

The modeling work presented here examined a rather simple and well behaved two-dimensional vertical slice problem. The average number of simulation time-steps needed to reach steady state was only about 27 and the model had an intermediate number of grid cells. We intend to test the limits of our method further by testing it on larger three-dimensional natural state problems. First we will consider synthetic test cases and after that move on to real case studies.

Over recent years typical grids for real natural state case studies have had up to an order of magnitude more grid blocks than was considered here (Austria & O'Sullivan, 2015; Gunnarsson *et al*., 2011; Kiryukhin & Miroshnik, 2012; Moon *et al*., 2014; Tateishi *et al*., 2015; Yeh *et al*., 2014). The general trend over the years has been an increase in number of elements, as computational resources have improved. Therefore, the forward Jacobian matrix will typically be larger for future applications, which will make evaluating a full sensitivity matrix more difficult. The model size is likely to affect what type of linear solver is most applicable for the analytical approach. As a result different linear solvers may need consideration for larger simulation grids for the analytical approach to work effectively. However, larger and more complex natural state problems tend to require a greater number of time-steps for convergence. This aspect will favor the analytical natural state approach, which only requires the solution for the final time-step of the steady state evaluation.

6. CONCLUSIONS

When using analytical methods, model sensitivities of steady state geothermal reservoir simulations can be evaluated quickly with modest computational resources. Employing the direct or adjoint sensitivity methods, computational effort required to find natural state model sensitivities can be expected to be number of simulation time-steps lower than the standard approach of using finite differencing. This is because numerous nonlinear transient forward simulations are avoided by using analytical differentiation of the steady state equations.

For a twelve parameter steady state inverse problem the analytical sensitivity approach gave results consistent with those found using finite differencing. Additionally the analytical scheme offered noticeable computational savings even for this small inverse problem. After confirming the applicability of the analytical approach a much larger 640 parameter natural state inverse problem was considered. As expected, applying the direct or adjoint analytical methods to a larger natural state inverse task resulted in a large reduction in

computational effort. Over a hundred computer processors would be needed to achieve similar results by parallelization of the finite difference method.

The natural state simulation problems considered in this work required a relatively small number of time-steps to converge to a steady state. Since the cost of the analytical sensitivity evaluations are independent of the number of simulation time-steps, we may anticipate considerable computational savings for more complicated models that require a large number of time-steps to reach a steady state (O'Sullivan *et al*., 2013, 2014).

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