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Accelerating the Solution of Geothermal Inverse Problems Using Adjoint Methods in Waiwera: Case Studies on Kerinci and Wairakei

Benjamin Gonzalez-Gutierrez[1], Ruanui Nicholson[1], John P. O'Sullivan[1], Angus Yeh[1], Elvar Bjarkason[2], Michael J. O'Sullivan[1] and Oliver J. Maclaren[1]

[1]Department of Engineering Science, The University of Auckland, Auckland 1010, New Zealand

[2]Institute of Fluid Science, Tohoku University, Sendai, 980-8577, Japan

ruanui.nicholson@auckland.ac.nz, oliver.maclaren@auckland.ac.nz

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ABSTRACT

The calibration of geothermal simulation models involves inferring the permeability structure of the system and the location of the deep upflow of heat and mass. Available data typically includes noisy temperature, pressure and enthalpy measurements from pre-existing wells.

Mathematically, model calibration is an ill-posed inverse problem. Solving such inverse problems typically involve minimising an objective or cost function that combines a measure of the fit of the model results to the available data, and a regularization term to overcome the ill-posedness or instability of the problem. Given sufficient computational resources, inverse problems can thus be formulated and solved as general constrained optimisation problems. These methods can require a large number of simulator runs, however, and large geothermal simulation models are typically computationally expensive.

Adjoint methods provide a method of speeding up the solution of inverse problems, provided model Jacobian information and other model derivatives are available. Adjoint methods can use this information to provide efficient evaluation of both first derivatives and second derivatives of the cost function. The gradient of the cost function can, for instance, be determined by running one nonlinear forward model simulation and one additional linear adjoint solve.

Here we discuss an application of the adjoint method to the calibration of models of the Kerinci and Wairakei geothermal fields, constructed in the new simulator Waiwera. Waiwera is based on an improved implementation of the same basic algorithm as TOUGH2, but with fully parallelised techniques and improved solvers. Most importantly for implementing the adjoint method, Waiwera also provides easy access to the model Jacobian.

1. INTRODUCTION

It is well-understood that the calibration of geothermal systems plays a fundamental role in both geothermal engineering and resource management (O'Sullivan, et al., 2001; O'Sullivan and O'Sullivan, 2016; Popineau, et al., 2018). It is also generally accepted that run-times for geothermal models (whether for natural state, production history, or future scenarios) can be prohibitive. Furthermore, this computational burden is often amplified when carrying out the calibration of the model, i.e., determining unknown parameters such as the permeability of the subsurface, or the location and/or magnitude of deep upflows.

Mathematically the process of calibration can be thought of as solving an ill-posed inverse problem (Aster et al., 2011; Engl et al., 1996), or a problem of statistical estimation (Evans and Stark, 2002; Stuart, 2010; Tarantola, 2005; Kaipio and Somersalo, 2006). Independently of how one interprets this process, the calibration process typically relies on the minimisation of a suitable cost function. The cost function includes a measure of the misfit between collected data (temperature, pressure, enthalpy etc.) and model outputs. Some form of regularisation is typically also required, due to the fact that the number of parameters to be estimated is often far more than the number of observations, the complex nature of the governing equations, and the fact that noise corrupts the measurements. Regularisation commonly takes the form of an explicit penalty term included in the cost function, which favours simpler models and/or models reflecting a priori expert knowledge. However, as discussed below, other forms of regularisation can suffice.

Model calibration can thus be framed generally as an optimisation problem, for which there are a number of well-understood solution methods. Several of the most efficient optimisation algorithms rely on the computation (or approximation) of first- and second-order derivatives of the cost function with respect to the unknown parameters. However, current state of the art automated geothermal calibration tools, such as iTOUGH2 (Finsterle, 2000) or PEST (Doherty, 2015), compute these derivatives using finite differencing (sometimes referred to as the perturbation method). This necessitates approximately the same number of (full, nonlinear) forward simulations as there are parameters at each step of the optimisation algorithm, which for many realistic geothermal models is infeasible.

The adjoint method, in many cases, allows for a considerable speed-up in the derivative calculation process. When the cost function is in the form of a sum of squares, using the adjoint method reduces the "per optimisation step" computation cost of the first derivative to one full nonlinear forward solve and one additional linearized forward solve. The required additional cost for second derivative evaluation is only in the form of linearized solves. The adjoint approach can be described as an effective use of the chain rule, which avoids inefficient or redundant computations involving the Jacobian matrix containing the derivatives of state variables, such as temperature and/or pressure, with respect to parameters of interest, such as permeabilities. The approach relies on knowledge of the model Jacobian, i.e., the derivatives of the governing equations with respect to state variables, and derivatives of the governing

equations with respect to parameters of interest. Given these, the cost function gradient, and/or the Jacobian itself, can be computed with minimal additional computational cost. This process is described in detail below.

The main aim of the current study is to bring together the past works of Bjarkason et al. (2014, 2015, 2016a, 2016b, 2019) on the use of adjoint methods in geothermal calibration with the use of the geothermal simulator Waiwera (Croucher, et al., 2016; Croucher, et al., 2018), and to apply these methods to models of real-world geothermal systems. A previous progress report on preliminary results from combining the adjoint method and Waiwera is given in (Gonzalez-Gutierrez et al., 2018). In that report we showed that, even for fairly small scale problems, use of the adjoint method can lead to large computational savings over automated calibration processes based on finite differencing. Since that report we have made significant progress.

To this end we present a brief overview of the adjoint method, and demonstrate its effectiveness at calibration for two real-world geothermal systems: Kerinci, Indonesia and Wairakei, New Zealand. To lower computational costs, and with the aim of good scalability, all simulations are carried out in Waiwera. While Waiwera solves the same governing equations as TOUGH2, it is highly parallelisable, implements improved solvers, and most importantly in terms of calibration with the adjoint method, offers easy access to the model Jacobian.

The paper is organised as follows. In Section 2 we recast the geothermal calibration problem as a mathematical inverse problem, and discuss standard optimisation procedures for solving it. In Section 3 we summarise the adjoint method, deriving the main equations, and show how it can be used for solving the geothermal calibration problem. In Section 4 we briefly review the current status of the new Waiwera geothermal simulator and comment on some of its key features. In Section 5 we show results for the calibration of the two geothermal systems, touching also on the problem of model run failures.

2. GEOTHERMAL CALIBRATION AND INVERSE PROBLEMS

The calibration of geothermal systems entails determining parameter values which give model output values in good agreement with collected data. Typical parameters include permeability, porosity, and deep upflows. Some of these parameters may not strongly influence calibration, but they may affect future predictions.

Calibrating a geothermal model is, in mathematical terms, equivalent to solving an inverse problem, or is, in statistical terms, equivalent to solving an estimation problem. The inverse problem is generally approached using constrained optimisation to obtain a point (best) estimate, and can be generically written as

$$\begin{aligned} &\min \quad f(\boldsymbol{u};\boldsymbol{p}) \\ &\text{such that} \quad \boldsymbol{g}(\boldsymbol{u};\boldsymbol{p}) = 0. \end{aligned} \tag{1}$$

Here f is the cost or objective function we wish to minimise, $\boldsymbol{u}$ is used to denote model output of measurable quantities, such as temperature or pressure, $\boldsymbol{p}$ are the parameters of interest, such as permeability or deep upflows, while the constraint $\boldsymbol{g}(\boldsymbol{u};\boldsymbol{p}) = 0$ represents the governing equations, that is, the combination of parameters and observables must satisfy the governing equations, i.e., nonlinear mass and energy transport equations and Darcy's law.

The objective function, f, most commonly takes a (generalised) least squares, or regularised least squares, form, i.e.

$$f(\boldsymbol{u};\boldsymbol{p}) = \frac{1}{2}\|\boldsymbol{W}_1(\boldsymbol{B}(\boldsymbol{u}) - \boldsymbol{d}_{obs})\|^2, \tag{2}$$

or

$$f_\alpha(\boldsymbol{u};\boldsymbol{p}) = \frac{1}{2}\|\boldsymbol{W}_1(\boldsymbol{B}(\boldsymbol{u}) - \boldsymbol{d}_{obs})\|^2 + \frac{\alpha}{2}\|\boldsymbol{W}_2(\boldsymbol{p} - \boldsymbol{p}_*)\|^2, \tag{3}$$

respectively. The matrices $\boldsymbol{W}_1$ and $\boldsymbol{W}_2$ are (usually predefined) weighting matrices, $\boldsymbol{B}(\cdot)$ is the observation operator which maps, for example, temperature throughout the computational domain to well locations, $\boldsymbol{d}_{obs}$ is the observed data, α is the regularisation parameter, and $\boldsymbol{p}_*$ is a reference value for the parameters (Aster et al., 2011). A cost function essentially the same as (3) can also be developed in the Bayesian statistics setting, assuming both the noise in the measurements and the prior distribution on the parameters are Gaussian (Tarantola, 2005; Kaipio and Somersalo, 2006; Stuart, 2010).

Regularisation of some sort is essentially a requirement for solving inverse problems (Engl et al., 1996), however the addition of an explicit penalty term to the objective function is not always required for regularisation, and alternative methods exist. One of the aims of regularisation is to avoid over-fitting of models to data, and can be achieved using strategies such as *early stopping*, as in the inverse problems (Engl et al., 1996) and machine learning communities (Orr and Müller, 2003), and so-called *regularisation-by-discretisation* (Kaipio and Somersalo, 2006; Aster et al., 2011).

Early stopping can be implemented by beginning the optimisation algorithm from a solution with *a priori* desirable properties, and only allowing the optimisation to proceed a limited number of steps away from this solution. This often naturally occurs in solving complex inverse problems using local search algorithms, as these often terminate in local optima well before overfitting can occur. The most important component in this approach is thus a physically plausible starting solution. A straightforward implementation of regularisation-by-discretisation in the context of geothermal inverse problems is to *a priori* specify the location and number of cell blocks within volumes composed of a single rock type, see Figures 2, 3, 5, or 6. This can be seen mathematically as projecting the unknown onto a predefined set of finite dimensional basis vectors, and can greatly reduce the dimensionality of the unknown parameters. Using these types of regularisation it may then be possible to solve the optimisation problem in (2) without requiring an explicit penalty.

2.1 Solving the Optimisation Problem

The solution to the inverse problem is the point in parameter space which minimise the associated cost function, i.e., (2) or (3). Stacking equation (3), leads to a problem of the same form as (2), thus, unless stated otherwise, here 'solving the minimisation problem' will refer to minimising (2), over parameter space. A large number of methods have been designed to carry out the minimisation of least squares problems such as (2). These methods include (Wright and Nocedal, 1999) steepest descent (SD), Gauss-Newton (GN), Levenberg-Marquardt (LM), and the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm. Both SD and BFGS only require the gradient of the cost function with respect to the parameters, on the other hand, GN and LM approximate the full Newton method Hessian using a method requiring the Jacobian matrix, i.e., the derivatives of the (discretised) state variables with respect to the (discretised) parameters (Wright and Nocedal, 1999).

As mentioned above, standard approach in the geothermal community for computing the required derivatives for model calibration is forward finite differencing. For example, in such an approach computing the (total) derivative of the cost function with respect to the requires solving

$$\frac{df(\boldsymbol{u};\boldsymbol{p})}{d\boldsymbol{p}_i} \approx \frac{f(\boldsymbol{u}(\boldsymbol{p}+h\boldsymbol{e}_i);\boldsymbol{p}+h\boldsymbol{e}_i) - f(\boldsymbol{u}(\boldsymbol{p});\boldsymbol{p})}{h} \tag{4}$$

for each $i \in N_p$, where N_p is the number of parameters, h is the step size, $\boldsymbol{e}_i$ is the unit vector in the i^{th} direction and $\boldsymbol{u}(\boldsymbol{p}+h\boldsymbol{e}_i)$ is the solution to the governing equations when perturbing the i^{th} parameter, i.e. $\boldsymbol{u}$ satisfying $\boldsymbol{g}(\boldsymbol{u};\boldsymbol{p}+h\boldsymbol{e}_i)=0$. As well as solving the N_p perturbed equations, forward finite differencing also requires the solution of the unperturbed equation $g(\boldsymbol{u};\boldsymbol{p})=0$. In the geothermal context, each of the N_p+1 simulations requires solving the full nonlinear forward problem. Thus, when forward simulations are computationally expensive, and/or when there are a large number of parameters to be found this can pose a severe obstacle. Moreover, finite differencing can give inaccurate approximations of derivatives, and often requires nontrivial scaling (Wright and Nocedal. 1999). A possible fix to avoid the inaccuracies is to use higher order finite differencing, however this adds considerably to the computational burden. Finite differencing can however be a useful tool for checking derivatives.

An alternative to the use of finite differencing for computing gradients and Jacobian matrices is the adjoint method (Bjarkason et al., 2014, 2015, 2016a, 2016b, 2019; Cao et al., 2003; Granzow, 2014; Gunzburger, 2003), discussed in the next section. The adjoint approach has been successfully applied to several fields of geophysics, but has only more recently been applied to geothermal calibration problems (for both natural state and production history), see e.g. (Bjarkason et al. 2014, 2015, 2016a, 2016b, 2019). However, these works used the TOUGH2 simulator and are based only on synthetic (two-dimensional) cases.

3. THE ADJOINT APPROACH

The adjoint method allows for the analytic computation of derivatives, and can be derived in a variety of ways (see, for example, Granzow, 2014). Here we derive the approach based on the method of Lagrange multipliers. Though we consider only the finite-dimensional (discrete) version, here, a similar approach is applicable in the infinite-dimensional setting (Nicholson et al., 2018).

To begin with, we introduce the Lagrange functional or simply a Lagrangian, which incorporates the constraints, i.e., satisfaction of the forward model, into an updated unconstrained objective function. The Lagrangian is given by

$$\mathcal{L}(\boldsymbol{u},\boldsymbol{p},\boldsymbol{\lambda}) \equiv f(\boldsymbol{u};\boldsymbol{p}) + \boldsymbol{\lambda}^T \boldsymbol{g}(\boldsymbol{u};\boldsymbol{p}), \tag{5}$$

where $\boldsymbol{\lambda}$ are so-called Lagrange multipliers, or *adjoint variables*. Although $\boldsymbol{g}$, $\boldsymbol{u}$, $\boldsymbol{p}$ and $\boldsymbol{\lambda}$ are all vectors, we will denote them now by g, u, p and λ, respectively, for convenience. Similarly, we will drop all other bolding of terms in the following.

It is well-known that at a constrained minimum of f all partial derivatives must vanish, i.e., , $\nabla_\lambda \mathcal{L}=0$, $\nabla_u \mathcal{L}=0$, and $\nabla_p \mathcal{L}=0$ (Wright and Nocedal, 1999). This requirement immediately leads to the following system of equations,

$$\begin{aligned} \nabla_\lambda \mathcal{L} &= g = 0 \\ \nabla_u \mathcal{L} &= \left(\frac{\partial g}{\partial u}\right)^T \lambda + \nabla_u f = 0 \\ \nabla_p \mathcal{L} &= \left(\frac{\partial g}{\partial p}\right)^T \lambda + \nabla_p f = 0, \end{aligned} \tag{6}$$

where we have used so-called *numerator* or *Jacobian* notation. The first equation of the system (6) ensures that at the minimum we also satisfy the forward problem. Rearranging the second equation gives

$$\left(\frac{\partial g}{\partial u}\right)^T \lambda = -\nabla_u f, \tag{7}$$

which is referred to as the *adjoint equation*, and is solved for the adjoint variables, λ. Equation (7) is in fact simply a linearised version of the forward problem, and thus far cheaper to solve than the full nonlinear forward problem $g(u;p)=0$. The final equation in the system (6), i.e.,

$$\nabla_p \mathcal{L} = \frac{\partial g}{\partial p}\lambda + \nabla_p f = 0, \tag{8}$$

states that the total derivative (gradient) of $\mathcal{L}$ with respect to parameters, p, is equal to zero at an optimum (in *parameter space*). Conversely, at points in parameter space away from an optimum, we have $\nabla_p \mathcal{L} = \frac{\partial g}{\partial p}\lambda + \nabla_p f \neq 0$, but which gives an efficient means to calculate the gradient. This can then be used for derivative based optimisation procedures.

As mentioned earlier, when using SD or the BFGS algorithm, it is only the gradient $\nabla_p \mathcal{L}$ which is required. However, for both the GN and LM algorithms we also require the Gauss-Newton (approximation to the) Hessian matrix, denoted by H_{GN}. The full Hessian matrix, H, is composed of the second derivatives of g with respect to parameters p. The Gauss-Newton approximation is usually favoured though, as it can be written in terms of the first-order Jacobian only and drops the (often hard to calculate) irreducibly second-order terms. Recalling that the cost function is in the (least squares) form of (2), the Gauss-Newton approximation is of then of the form

$$H_{GN} = \left(\frac{\partial\left(W_1(B(u) - d_{obs})\right)}{\partial p}\right)^T \left(\frac{\partial\left(W_1(B(u) - d_{obs})\right)}{\partial p}\right) = \left(\frac{\partial\left(B(u)\right)}{\partial p}\right)^T {W_1}^T W_1 \left(\frac{\partial\left(B(u)\right)}{\partial p}\right). \tag{9}$$

The observation operator, B, is often (and in our case) taken to be some kind of interpolation operator, giving only state variable values at observation locations, and is thus linear and independent of both u and p. This means we can rewrite the Gauss-Newton approximation as

$$H_{GN} = \left(\frac{\partial u}{\partial p}\right)^T B^T {W_1}^T W_1 B \frac{\partial u}{\partial p} = J^T B^T {W_1}^T W_1 B J, \tag{10}$$

where $J = \frac{\partial u}{\partial p}$ is referred to as the Jacobian matrix. Noting that $\nabla_p \mathcal{L}$ and the *total derivative* of f with respect to the parameters p must coincide, it can be shown that the Jacobian is of the form

$$J = \left(\frac{\partial g}{\partial u}\right)^{-1} \frac{\partial g}{\partial p}. \tag{11}$$

It is worth noting that although in this work we compute J by solving (11) as a linear system with multiple right-hand sides, i.e. as a linear system of the form $\left(\frac{\partial g}{\partial u}\right) J = \frac{\partial g}{\partial p}$, this need not be the case. In fact, for extremely large scale problems direct calculation of J may need to be avoided. In such cases iterative methods such as (preconditioned) conjugate gradients (CG) or randomised truncated singular value decomposition (RTSVD) methods (Bjarkason et al., 2018) may be required.

To carry out the adjoint method we thus require the following four partial derivatives:

- The model Jacobian, $\frac{\partial g}{\partial u}$: This matrix is in fact used to solve the nonlinear forward simulations, and is easily set as an output in Waiwera, as discussed in Section 4.
- Governing equations with respect to parameters, $\frac{\partial g}{\partial p}$: This matrix can be derived analytically, as shown by Bjarkason et al., (2014, 2015, 2016b, 2019). Alternatively, in the future it may be possible to access these terms directly from Waiwera.
- The cost function with respect to state variables, $\nabla_u f$: This straightforward to compute,

$$\nabla_u f = B^T W_1^T W_1 (Bu - d_{obs}). \tag{12}$$

- The cost function with respect to parameters, $\nabla_p f$: This is also typically straightforward to compute, however it depends on what type of regularisation is used. If regularisation is used such as in (3), we have

$$\nabla_p f = \alpha W_2^T W_2 (p - p_*). \tag{13}$$

4. THE WAIWERA SIMULATOR

Waiwera was developed, and continues to be developed, at the University of Auckland, New Zealand. Waiwera is based in large part on existing geothermal simulation tools such as TOUGH2/(AU)TOUGH2 (Pruess et al., 1999; Yeh et al., 2012). Computationally, the benefits of using Waiwera for geothermal model simulations, as opposed to TOUGH2, are the parallel capabilities and access to additional solvers. Furthermore, Waiwera has improved methods for computing the model Jacobian (Croucher et al., 2018), which is pertinent to the use of adjoint methods.

Waiwera has been evaluated on various benchmark test cases, based on the Geothermal Model Inter-comparison Study (Croucher, et al., 2016; Croucher et al., 2018). These include a 3-D reservoir flow simulation and full-scale natural state simulations of a model of the Ngawha geothermal system, Ngawha, Northland, New Zealand. In a majority of the benchmark tests, Waiwera performed as well as, or better than, the industry-standard TOUGH2, measured in terms of scalability to large problems, time taken for solution convergence and whether or not the simulator converged in a predefined number of iterations. As an example of the possible speed up in computations, some models which would require days of simulation time in TOUGH2 to converge could be solved in hours using Waiwera (Croucher et al., 2018).

In the context of automated model calibration, another benefit of using Waiwera is the ease of access to model Jacobian matrices, which are required for the adjoint method (see Section 3 above). This goes a long way in negating the need for manual intervention, which is generally required to carry out the same calculations in TOUGH2.

5. CASE STUDIES

Here we discuss the results for the calibration of two geothermal systems, namely Kerinci, in Sumatra, Indonesia, and Wairakei, in the Taupo Volcanic Zone (TVZ), New Zealand. Models of both these systems have previously undergone significant manual calibration, see for example (Prastika et al., 2016) and (O'Sullivan et al., 2009, Yeh et al., 2018), respectively. To assess performance, we compare the results obtained using the adjoint method to those obtained after manual calibration. The parameters inferred are the x-, y-, and z-components of the permeability for all of the rock types along with the strengths of deep upflows. As is standard in geothermal calibration problems we assume the rock-type boundaries are fixed (and known) *a priori*, along with the locations of the deep sources. This approach provides a form of regularisation-by-discretisation, as discussed above. Furthermore, for both examples, optimisation using the adjoint approach was carried out using the Gauss-Newton algorithm, implemented via the Python SciPy library (Jones et al., 2001).

5.1 Kerinci

As an initial test problem we consider the calibration of a relatively coarsely discretised geothermal model of Kerinci, Sumatra, Indonesia. This has a total of 908 blocks, including one layer (56 blocks) of atmospheric blocks, see Figures 2 and 3. The model consists of 10 rock types and contains 4 deep sources, leading to a total of $N_p = 10 \times 3 + 4 = 34$ parameters to be estimated. Typical (well-behaved) run times for the nonlinear forward model using Waiwera (in serial) are in the order of 1 second, while linear solves are effectively free, thus providing an efficient means of testing the method. Data for the model consists of 79 temperature measurements distributed at three separate wells. However, the wells are clustered near the centre of the model and occupy very few cells.

Using the default settings for Gauss-Newton in the SciPy library, the optimisation converged in 71 steps. The temperature data, the temperature outputs at wells after manual calibration and the temperature outputs at wells after calibration using the adjoint method are shown in Figure 1 for the three wells. Model temperature outputs appear coarse due to interpolation. The automated calibration of the Kerinci model using Waiwera and the adjoint approach appears to be fairly robust to selection of the initial parameter values. That is, by setting any fairly reasonable initial guesses for the parameters the optimisation method converged to essentially the same calibrated parameter values.

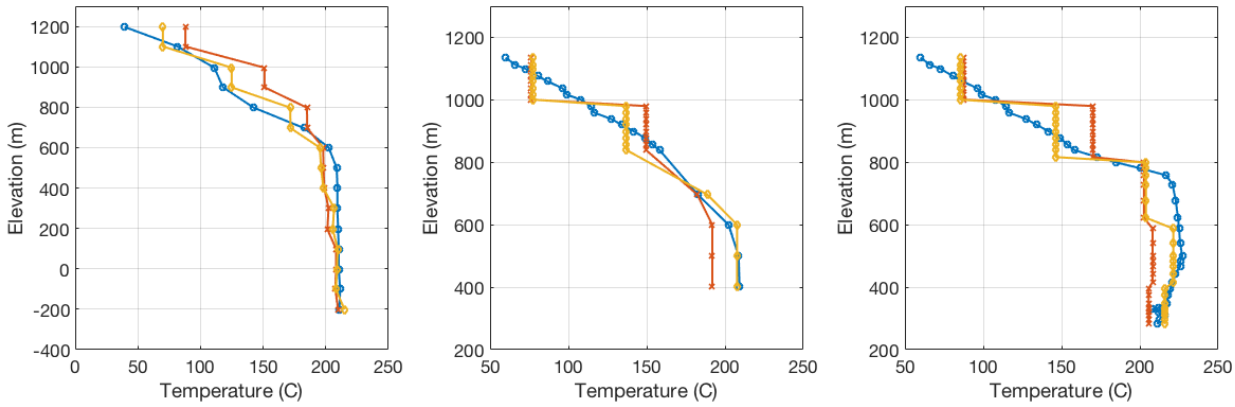

Figure 1: Temperature data (blue), manually calibrated temperature output (red) and automated adjoint based calibration temperature output (yellow) for Kerinci down the three wells.

From examining the misfit in data, it is quite clear that the adjoint approach outperforms manual calibration. More specifically, when using the adjoint approach we are able to reduce the objective function to 1.43×10^4, while conversely, the objective function value is 3.17×10^4 after manual calibration. In Figures 2 and 3 we show the x-component of the permeabilities along a vertical slice after manual and adjoint based calibration, respectively. The adjoint method achieves better fits to the data while simultaneously maintaining physically reasonable and meaningful parameter estimates.

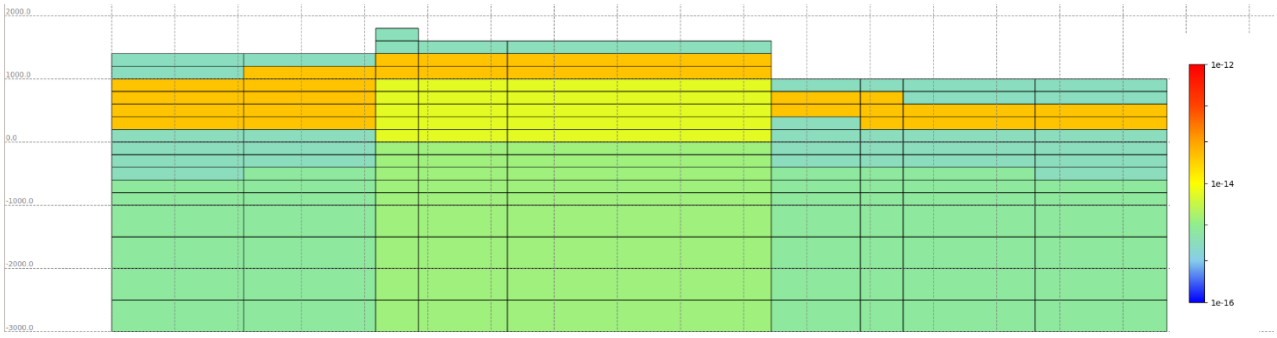

Figure 2: Kerinci vertical slice showing x-component permeability after manual calibration.

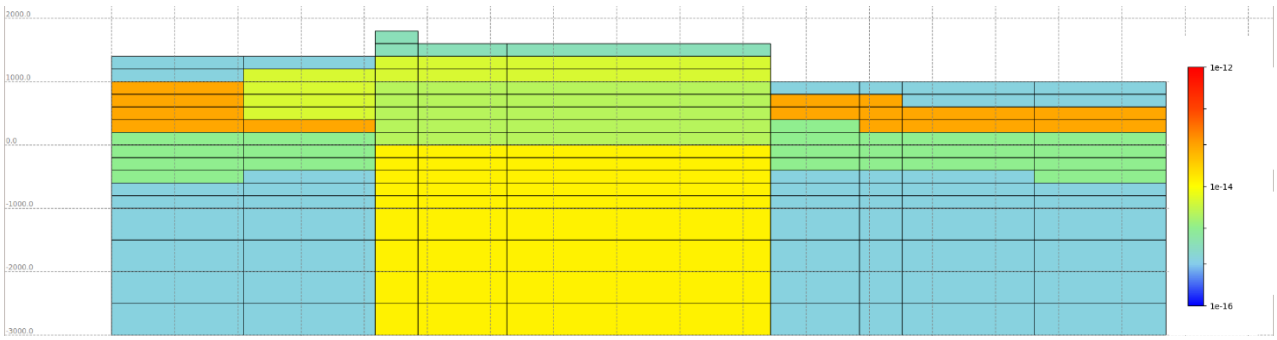

Figure 3: Kerinci vertical slice showing x-component permeability after automated adjoint based calibration.

5.2 Wairakei

As a more challenging problem, we consider calibration of a geothermal model of Wairakei, TVZ, New Zealand. The model has 38,876 blocks inclusive of 1,020 atmospheric blocks. The parameters to be estimated are the three permeability components of 121 rock types and the strength of 84 deep sources. Thus the total number of parameters is $N_p = 121 \times 3 + 84 = 487$. Run times for the nonlinear forward Wairakei model using Waiwera (in serial) varied from 2 minutes to 20 minutes. As with the Kerinci example, the linear solves are effectively free. Field data used for calibration are 3,977 temperature measurements distributed at 37 wells located throughout the model. In contrast to the Kerinci model, the well locations are well-distributed throughout the computational domain.

With adjoint approach, the optimisation procedure managed 7 updates before so-called *model run failures* became a major difficulty, as discussed below. Model run failures also became problematic when the initial estimate for the parameters were set arbitrarily. This resulted in manually calibrated parameter values being set as the initial parameter estimates for the adjoint method. Temperature data from 3 wells along with the relevant temperature outputs after manual calibration and the relevant temperature outputs after the 7 parameter updates using the adjoint approach are shown in Figure 4. The coarse appearance of temperature outputs from the models is due interpolation. Model failures have also been an ongoing issue in using manual calibration methods, and appear to reflect the properties of the model itself, rather than the calibration method.

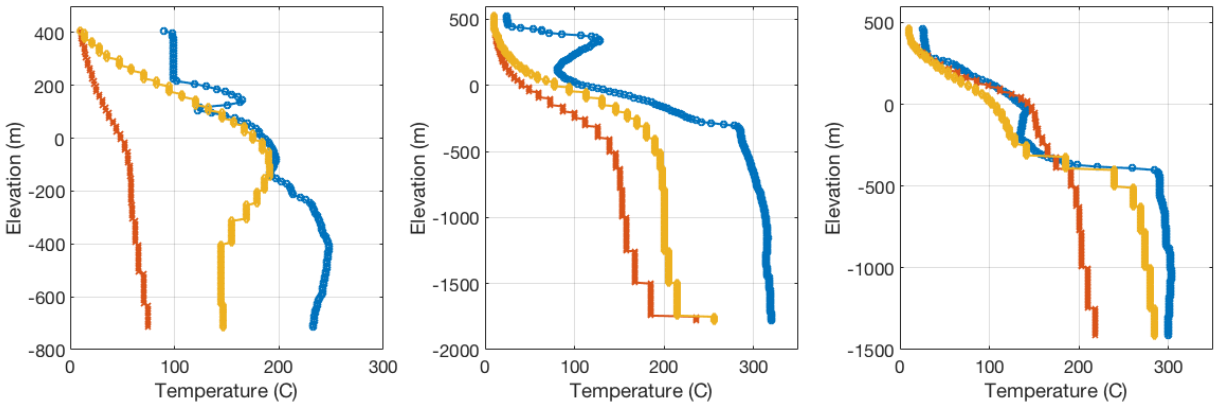

Figure 4: Temperature data (blue), manually calibrated temperature output (red) and automated adjoint based calibration temperature output (yellow) for the wells in the Wairakei geothermal model

In Figure 4 we see a significant improvement in fitting the data when using the adjoint approach as opposed to manual calibration. The objection function value for the manually calibrated model is 3.17×10^7, while for the calibration carried out using the adjoint method the objective function was lowered to 1.82×10^7, thus quantifying the improvement gained by using the adjoint method. In Figures 5 and 6 we show the x-component of the permeabilities along a vertical slice after manual and adjoint based calibration, respectively. Importantly, as in the Kerinci case, the parameter values found using the adjoint method are physically plausible.

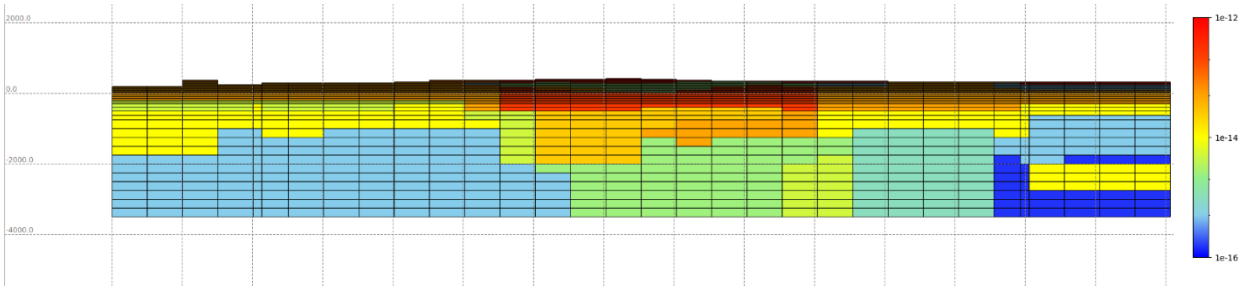

Figure 5: Wairakei vertical slice showing x-component permeability after manual calibration.

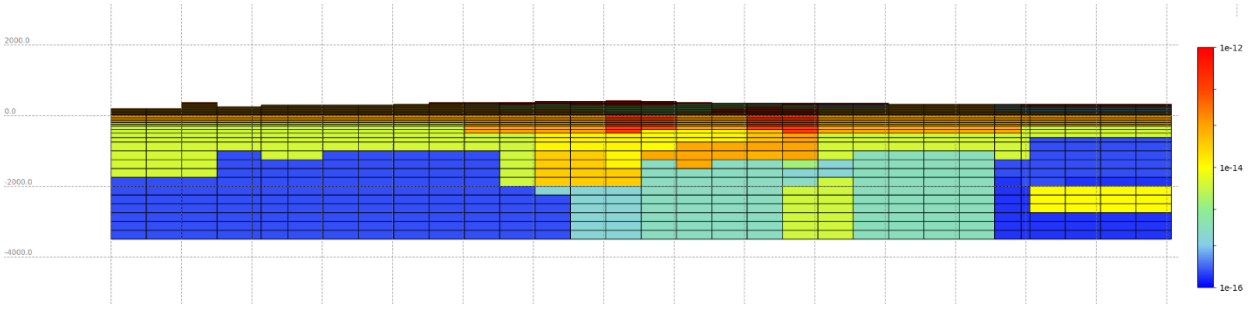

Figure 6: Wairakei vertical slice showing x-component permeability after automated adjoint based calibration.

5.2.1 Model Run Failures

Simulator run failures have been an ongoing issue when calibrating the Wairakei model, whether manually or via automated methods. This has also been an issue with other complex geothermal models. Though there are cases in which Waiwera is able to complete natural state model runs while TOUGH2 simply will not converge, there are also cases for which model run failures appear to be independent of the simulator. Model run failures, in the context of geothermal natural state model runs, arise when the simulator cannot achieve a user defined threshold for the minimum time step length when carrying out *time marching*. In simple terms, the simulator cannot find a *steady state*. There are several factors which can contribute to model run failures. Of particular relevance to the calibration process is the problem that small changes in (seemingly innocuous) parameters, for example the x-component of the permeability for a specific rock type far from deep upflows, result in model run failures. This indicates that significant effort in understanding the *forward* problem is still required.

6. CONCLUSIONS

In this work we have shown that the adjoint approach provides an attractive method for carrying out automated calibration of geothermal models. We demonstrated good improvement over manual calibration for models of two real-world geothermal systems, Kerinci, Sumatra, Indonesia and Wairakei, TVZ, New Zealand, and our approach requires much less user input. In both cases the objection function was substantially reduced, while maintaining plausible parameter values.

The adjoint method fits especially well with the capabilities of the (still in development) Waiwera geothermal simulator, as this simulator offers easy access to model Jacobians which are essential to the adjoint approach. Furthermore, the Waiwera simulator is particularly well suited to large-scale problems, and the adjoint methodology generally scales very well to such problems, with derivative computation costs essentially independent of the number of parameters. Thus the combination of improved large-scale forward simulation and adjoint methods for large-scale inverse problems should be appealing for geothermal modellers. On the other hand, the framework laid out in this paper is essentially independent of which geothermal simulator is used, and has also been used successfully alongside the TOUGH2 simulator.

Further work is required to ensure the methods outlined in the current paper can be easily used in practice, however. Firstly, the issue of model run failures in the context of calibration is a key challenge. This may require the use of techniques from stochastic optimisation for solving the inverse problem, methods for identifying *a priori* which models are likely to run well, and/or require additional work on the forward problem.

The calibrations carried out in this paper focused on finding a single (best) estimate of the parameters of interest, although it is often useful to have some measure of the associated uncertainty in the parameter estimates. Thus, future work includes the incorporation of so-called *uncertainty quantification*. Efficient derivative computation is again very useful for this, and the adjoint methodology will likely play a key role. Furthermore, here we have presented calibration results for the natural state only; however, the adjoint method can allow for production history calibration, and thus we intend accommodate this feature.

Finally, though the use rock types made up of multiple cell blocks is standard in geothermal modelling, the framework laid out in this study can be extended to the case of every cell block being an individual rock type. This most likely will require more careful regularisation strategies, however, to ensure that physically plausible rock structures are preserved during optimisation.

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