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Geothermal Supermodels: the Next Generation of Integrated Geophysical, Chemical and Flow Simulation Modelling Tools

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ABSTRACT

Existing geothermal modelling tools were designed over 25 years ago and are increasingly unable to cope with modern demands, both in computational practicality and in resolving scientific and resource specific questions. Today, numerical models are used for financial project planning and geothermal field management, and are required to be considerably more detailed than previous generations of models.

This paper presents a four-year, New Zealand-based, research programme that seeks to develop next generation integrated geothermal modelling tools, including a new flow simulator, geophysical and geochemical codes, and the linkages between them. This ambitious advancement will add capability through the integration of information from different disciplines, and overcome some of the limitations of current modelling software.

There are two major foci of the programme: the development of a new reservoir flow simulator; and integration of models from different disciplines. A modular approach will see the first stage developing a next-generation geothermal simulator using state-of-the-art numerical techniques. The key priority is to develop core functionality and provide frameworks to allow more complex descriptions of different reservoir processes to be incorporated later.

The second stage involves developing improved numerical methods and modules to couple key processes, including reservoir flow, geophysical, geo-mechanical, geological, groundwater and geochemical models. This research will provide improved models of geothermal processes (e.g. fluid flow), structures (e.g. faults) and conditions (e.g. supercritical temperature), enhancing the ability of developers and users to model the wide range of conditions seen in geothermal reservoirs.

1. INTRODUCTION

Computational science is defined as a rapidly growing multidisciplinary field that uses advanced computing capabilities to understand and solve complex problems (Benioff and Lazowska, 2005). This area is becoming the third pillar, or leg, of science alongside the traditional pillars of theory and experimentation (Kolda, 2014). For geothermal activities, computational modelling offers unprecedented opportunities to:

- Understand regional scale processes controlling flows in geothermal systems
- Assess the potential of fields for electricity generation
- Predict the impact of geothermal developments on the environment
- Estimate the costs associated with a geothermal development

In order to make the most of these opportunities, significant advances are required in the software and techniques that are used for modelling geothermal systems. The geothermal modelling community is full of capable and inventive people, but progress is being hindered by the lack of modern, universally accepted software and techniques. As an example, a common requirement of models of development systems is the estimation of future makeup well numbers. But such a conceptually simple requirement cannot be easily obtained from the most commonly used simulator for production field modelling, TOUGH2 (Pruess, 1991) as it does not accommodate automatic turning on of production wells. (There are variants of TOUGH2 that include this feature, but these are not trivial changes to the code).

The Reservoir Modelling Working Group of the International Partnership for Geothermal Technology (IPGT 2012) issued a report on research and development themes for future geothermal modelling. This includes a goal of reliable software tools aiding decision making in engineering, managing and optimizing geothermal reservoirs by 2020. They illustrated this goal with the diagram shown in Figure 1. While we agree with the broad approach suggested, it is important, in our view, to ensure that issues related to practical geothermal reservoir modelling in the 21st century are also addressed. These issues commonly arise from industry models of development systems and include:

- Improving reliability so that reasonable models run to completion
- Calibration of models with little to no data from drilled wells
- Coupling reservoir models with existing chemistry or mechanical models.
- Coupling reservoir, wellbore and plant models.

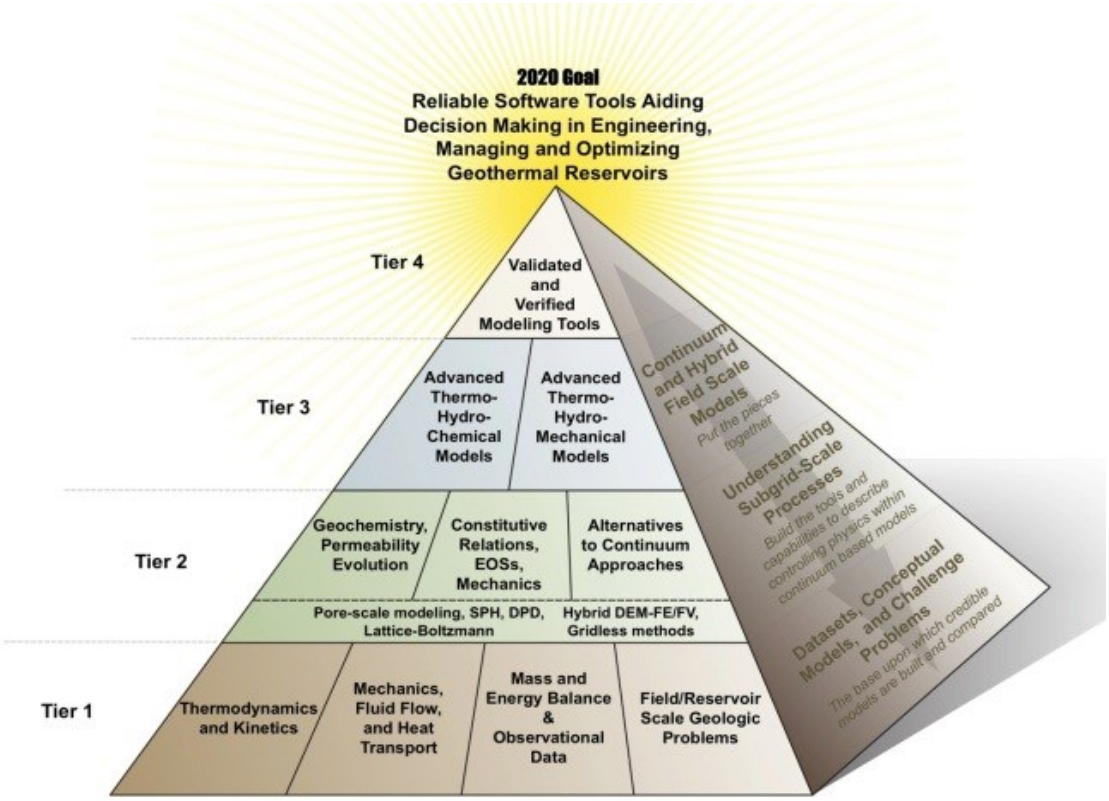

Figure 1: IGPT Technology Development Pyramid for reaching a 2020 goal of fully coupled thermo-hydro-mechanical-chemical simulators for predicting short- and long-term production capacity in hydrothermal and enhanced geothermal reservoirs.

Individual groups are currently working in these areas: developing new codes (PFlotran, FALCON, OpenGeoSys); and adding couplings to existing codes (Hernandez et al, 2015). But the approaches are typically individual and uncoordinated. Our group has been successful in obtaining funding for a four-year, New Zealand-based research programme, called "Geothermal Supermodels", to focus on the topic "To better understand and model multiple geothermal systems, the interactions between them and their sustainability through the use of geophysical, geochemical, and in particular, numerical modelling tools". A key part of this programme is the development of software and techniques to improve our ability to model geothermal systems. Our aim is to provide the industry with robust and flexible software that can meet the needs of the foreseeable future.

2. EXISTING MODELLING TOOLS

The geothermal industry has a thriving research sector which has developed a number of software codes for modelling purposes. Some of these codes have become widely used within the industry and are commercially available (for example TOUGH2, and Geochemist Workbench). Typically these codes have a long history, but also have designs rooted in the 1980s. Other, more modern, codes are focused on specific problems (SULEC), have designs that make extensions difficult (DuMux is template driven C++) or are mainly used by individual researchers (FALCON). Very few of these codes focus on the flexibility and robustness required by the geothermal industry, nor do they attempt to integrate models from different disciplines.

Limitations in the existing numerical, geophysical and chemical modelling tools have challenged the geothermal industry and research community for the last 10+ years. Too much effort is spent attempting to overcome these limitations in order to address current day issues. These limitations involve both computational practicality and applicability of codes to particular questions.

An example of the limitations of existing codes is seen in the problem of modelling the hydrothermal alteration seen in many shallow capping structures of geothermal systems (for example see Clearwater et al, 2011). This requires at least a thermo-hydro-chemical (THC) model with transport of water, energy and chemical species, phase changing, chemical reactions and porosity/permeability alteration. Reactive transport codes such as ChemTough (White, 1995) and ToughReact (Xu et al, 2004) can include all these aspects in a model. But for the timescales of many thousands of years and the length scales of kilometres, the computation time for these codes is prohibitively long. For this model, the important changes in chemistry occur in a relatively small volume. The ideal solution technique would involve a detailed reactive transport model in the upper few hundred metres coupled with a coarser (in space and time) model over the rest of the system. But attempting to retrofit such a model on existing codes such as ChemTough, ToughReact or TOUGH2 would be very difficult and require rewriting substantial portions of the code.

A second illustration of the limitations of the existing codes is the number of papers presented at industry conferences on modifying TOUGH2 to either circumvent underlying issues or to extend the code's capabilities. Over the last two Stanford Workshops on Geothermal Reservoir Engineering and New Zealand Geothermal Workshops a total of eight papers have been presented on these

topics (Croucher and O'Sullivan, 2013, O'Sullivan et al, 2013a, Nandanwar and Anderson, 2014, Kiryukhin et al 2014, Xiong et al, 2013, Peluchette and Anderson, 2013, O'Sullivan et al, 2013b, Gudmundsdottir et al, 2013). Extensions of TOUGH2 have developed by many groups, but they are typically difficult to implement and this leads to ad-hoc solutions and unreliable models.

TOUGH2 (Pruess, 1991) has been a success story for the geothermal modelling community, and has been widely adopted for geothermal reservoir modelling and many other applications. This success is due to a combination of factors including availability at a relatively low cost with full access to source code and design decisions that allowed limited extensions to the code. However it is written in an old-fashioned style of FORTRAN and is quite difficult to modify the internal sections of the code and was never designed to address many of the detailed questions that are being posed of today's reservoir models.

Continuing to patch the standard tools will not provide the geothermal community with the robustness required for the 21st century. New methods are needed to model deep to near surface heat-mass flow systems and linkages between individual geothermal systems that have proven difficult to resolve using dated non-integrated, reservoir, geophysical and chemical modelling approaches.

3. THE "GEOTHERMAL SUPERMODELS" APPROACH

For the reasons outlined above, we believe that the time has come to develop numerical modelling tools and methodologies that will serve the needs of industry and researchers in the early part of the 21st century. Using research funding from the NZ government, we have developed a programme to start this development.

A key priority is to develop core functionality in the reservoir simulator and provide frameworks to allow more complex descriptions of reservoir processes to be incorporated later. That is, substantial flexibility will be incorporated in the design phase. We will combine modern modular coding techniques with the years of knowledge and specialist know-how that exists in the geothermal sector. A key advantage of the modular approach is allowing users to include or exclude particular modules as required and to extend the simulator as needed in the future. This approach also allows researchers to work independently on specific modules with a clear interface to the core flow models developed through this programme.

The guiding principles for this development are flexibility and robustness. Flexibility will enable researchers to extend the capabilities of the simulator without needing to understand every line of code in the core of the software. Robustness is essential as "reasonable" models need to run and produce results – which is not the case with many of the current codes.

We seek collaboration with other groups around the world, and it is our intention to provide this software through an open source license. For our vision to come to fruition, we need to engage a critical mass of users. As well as working with the research community; it is our intention to work closely with the geothermal industry in NZ and overseas to provide a robust tool that can be used in the commercial environment.

The programme splits naturally into 2 parts: one focused on numerical methods and code development; the other is focused on modelling key reservoir processes including coupling and validation.

4. CORE GEOTHERMAL RESERVOIR NUMERICS

The design of the programme involves a core flow simulator that can be extended easily using modules. Requirements of this core simulator are:

- robustness;
- computational efficiency;
- ability for parallelization;
- flexible model grids,
- flexible boundary conditions,
- flexible model wells

This flow simulator will be designed to handle large-scale complex models involving multiple, interconnected geothermal systems.

4.1 Core Simulator

The programme provides an opportunity to utilize modern numerical methods together with modern coding practices. In terms of computational efficiency, parallelization offers the greatest prospect to speed up calculations. The computational speed of the numerical modelling software currently used by the geothermal industry and researchers can be prohibitively slow. For example calculations of a single geothermal system represented by 50,000-100,000 elements can sometimes taking weeks to complete. Much faster computational speed is required to carry out extensive numerical experiments with the large and complex models required to represent multiple systems (possibly an order of magnitude larger than existing single field models).

The code will be designed to work with libraries of parallel linear solvers such as PETSC or Paralution. We will test various approaches for applying domain decomposition, and also test different approaches to parallelization. Algorithms designed for small shared memory systems may be suitable for many problems and can exploit characteristics of the problem – for example in a dual porosity system, the fracture and matrix systems can be treated on separate processors. For many problems, speed ups of 5 to 10 will be sufficient. On the other hand, very large problems may require generic algorithms that can be applied to massively parallel supercomputers.

Other areas offer opportunities to make a significant impact on the computational speed of geothermal flow models exploiting specific features of geothermal models (Yeh et el, 2011 and Croucher et al, 2004). One of the most time consuming modelling tasks is getting a natural state model to run to a steady state. We aim to:

- Test direct solutions of the nonlinear steady flow equations as an alternative to using a transient approach to reach a steady state
- Produce robust and efficient phase change algorithms that overcome existing issues of handling phase transition in the presence of multiple chemical components

The core computational task for a geothermal simulator is the solution of the large number of coupled, nonlinear, mass and energy balance equations. This is an iterative procedure, where at each stage we need to solve a large set of linear equations, and this is the key step that can limit the speed of the simulation. We aim to determine the most efficient linear equation solvers and pre-conditioners, and optimum domain decomposition algorithms. This will be done by extensive testing on a range of sample problems known to be numerically challenging.

We will develop new modules for the flow simulator to couple with key processes (e.g. chemistry, fracture flow, rock mechanics). A common approach will be (i) developing a framework for coupling into the simulator; and then (ii) developing specific modules using that framework.

4.2 Equations of State

Equations of State (EOS) routines provide the basic fluid properties which are used by a flow simulator to formulate the nonlinear conservation equations that govern fluid, heat and chemical flows within a geothermal system. For example, the EOS routine for pure water must provide the density, enthalpy and viscosity as a function of the pressure and temperature. If additional chemical species or multiple phases exist, then the mass fraction of the chemical or the volume fraction of the phases are required to describe the thermodynamic state of the fluid.

Existing EOS modules such as those used in TOUGH2 cover a range of components (e.g. salt, air, hydrogen, CO_2), but each has its own method of specifying the fluid properties and phase transitions. We propose to overcome the complexity introduced by this approach by developing a new EOS framework with a consistent approach to treating components and phases. We will utilise existing modern formulations of water properties (IAPWS, 1995 and IAPWS 1997) as the core of this work. Key requirements of this framework are:

- Ensuring that the nonlinear features of the phase diagram do not prevent convergence of models.
- Optimisation of performance, as these calculations are executed many times during a simulation.

It is crucial that the EOS framework seamlessly allows supercritical conditions to be modelled, as models seek to include deeper, higher temperature regions.

4.3 Fracture Flow

Flow through fractures and other high permeability pathways are important processes in geothermal systems. Many current approaches to incorporating fracture systems into models, such as MINC (Pruess, 1992), are simplified and do not represent the full complexity of flow paths found in geothermal systems. They are often based on 50 year old concepts from the oil and gas industry (Barenblatt et al 1960, Warren and Root, 1963). Additionally, these approaches do not take advantage of the special character of a fractured system. For example, heat and mass transfer from matrix to fracture is likely to be a slower process compared to transport in the fractures. This offers the opportunity to develop iterative schemes that work alongside the standard Newton solvers.

We aim to better model these high permeability flows by developing a framework for representing fast flow paths in the reservoir. The framework will allow for:

- Flows to be calculated on different time scales from those in the full reservoir model,
- Coupling fast flow paths to different parts of the reservoir,
- Geometrical effects (e.g. fault orientation and regions where fractures are sparsely distributed) to be incorporated into the model,
- Improved and realistic representations of fracture processes.

We will build on recent innovations in modelling flow in fractured media (Geiger et al, 2013, Moinfar, 2013).

4.4 Chemistry

Chemistry is an essential element for modelling geothermal systems and processes. Existing approaches for incorporating chemistry into geothermal simulators are limited to adding chemical species to model changes in fluid properties and track concentrations, considering only deposition and dissolution processes, or calculating the full chemical environment using large sets of chemical species (e.g. reactive transport codes such as ChemTough, ToughReact). The first approach is too simple for most applications, but the reactive transport codes are computationally expensive and are not suitable for modelling naturally occurring geothermal systems and their environs over typical timespans of interest.

What is required is a method that captures the key chemical reactions and is computationally feasible. We will develop a new framework for incorporating chemical species into the flow simulator that will calculate changes in fluid properties due to different species concentrations, transport of species under the flow field and concentration changes due to reactions. We will develop new chemistry modules based on small sets of species that control key chemical properties. A corresponding set of equations that approximately describe the reactions will be developed and this system will be coupled to the flow simulator using the new chemistry framework. This could, for example, allow the tracking of solution pH without the need to solve all of the equilibrium equations at each timestep.

4.5 Rock Mechanics

Thermo-hydro-mechanical (THM) models that calculate the stress state are important for understanding the behaviour of natural geothermal systems such as: how heat and mass are transferred through the deep (>6 km) brittle/ductile transition zone; how large-scale geological structures affect the location and nature of geothermal systems; and interactions between neighbouring geothermal systems. On a smaller scale, THM models are also important for understanding how the injection of cold water affects permeability surrounding an injection well, and how geothermal developments impact the surface (e.g. subsidence).

Existing geothermal models are limited in their ability to account for THM behaviour. We will develop a framework for coupling geo-mechanical models to the flow simulator. We aim to determine the level of coupling that is required for simulating THM effects on heat and mass transfer. This will be assisted by laboratory studies to define rock properties at high pressures and temperature. Initial steps will also be undertaken to introduce chemical effects, for example mineral deposition or dissolution that affect permeability and porosity.

5. COUPLING AND VALIDATING RESERVOIR MODELS

In addition to the need for better software for geothermal modelling, there is a need for improved coupling and validation techniques. A typical reservoir model will incorporate information from geology, geophysics and geochemistry into the model structure. But often this information is used as input data (e.g. rock types, MT boundary) or as calibration data (chloride or gravity changes). Access to supercomputers means that higher levels of coupling between disciplines can be considered. This becomes particularly important when modelling regions where drilling has not occurred.

The coupling of different model types (flow, geophysical, mechanical and chemical) will provide improved developer and regulator confidence in both development and validation of models, and the chemical and thermodynamic processes that occur in them.

5.1 Inverse Modelling

Inverse modelling is an important part of the validation process. Many models require estimation of parameters that cannot be directly measured, e.g. rock permeabilities and porosities. Inverse modelling is an established method for undertaking this estimation. In the geothermal context, it also provides a means for systematic investigation of conceptual models of sectors of the system where data are sparse.

Basic inverse modelling techniques have been developed and are well implemented by a number of groups (e.g. PEST and iTOUGH2), but these packages can only optimise model parameters given a particular geological model and rock-type assignment within the reservoir model and this is never precisely known. We will develop a controlling heuristic code that uses nonlinear optimisation techniques to experiment with rock-type assignment in a systematic fashion, and interfaces with other inverse modelling codes.

5.2 Geophysical modelling

As part of an existing research project that guides future deep geothermal exploration in the Taupo Volcanic Zone (TVZ) of New Zealand, seismological and magnetotelluric (MT) measurements have been made to investigate the nature and structure of geothermal systems below the depth currently being exploited for power production. Results from this programme have, for the first-time, imaged the connections between conventionally drilled and developed TVZ geothermal systems, i.e. 2-3 km depth range, and their underlying magmatic heat source. However, the non-proprietary methods of MT data inversion (Siripunvaraporn, 2005 and Egbert and Kelbert, 2012) used for this work are cumbersome (e.g. MT data inversions may take several months to complete). This makes the resolution studies needed for model verification very difficult to undertake.

We propose to develop a new boundary integral (Benites and Aki, 1994, Benites et al 1997) approach to geophysical data inversion, which should reduce the computational burden by representing the model as a series of surfaces or interfaces separating regions with different properties, rather than as a 3D grid of small elements. The latter conventional approach results in the number of unknown model parameters being far in excess of the number of data available to constrain the model. An interface based approach would greatly reduce the degree of over-parameterization and allow model sensitivities to be calculated more efficiently. This approach will also make detailed resolution studies practicable and make the incorporation of geological information and interactive hypothesis testing easier.

5.3 Geo-mechanical modelling

Magma bodies and partial melt residing below geothermal systems are believed to have a profound effect on the stress distribution and thus fracture distribution in the surrounding brittle regions of the crust, providing the flow paths for the geothermal fluid (Kissling and Ellis, 2011). We aim to improve and optimise an existing code (Ellis et al, 2007, Ellis et al, 2011) to provide efficient solutions to 3D mechanical problems, including partial melt. We will develop an intuitive interface to incorporate geological and geophysical data, regional fault structure, and far-field tectonic forcing of the system in order to constrain the 3D regional geo-mechanical model. This model will include zones of partial melt (constrained by MT), brittle and ductile processes (constrained by seismology and rock properties), geological structure and regional tectonic forces. It will also be combined with a regional scale 3D model of the overlying hydrothermal fluid flow system to provide boundary conditions, stress conditions, fluid and heat inputs, and other constraints for smaller, field-scale geothermal models.

5.4 Groundwater coupling

Linking shallow groundwater models with deep geothermal reservoir models can be important in understanding how changes in the geothermal field (e.g. pressure decline) can influence shallow hydrological conditions. For example changes in geothermal pressures can reduce flows to surface features or can induce cold downflows which cool the reservoir. While sophisticated groundwater models have been created for many areas (Rosen and White, 2001), direct coupling to deep geothermal reservoir

models is not generally feasible due to a lack of simple, efficient coupling tools. The new capabilities of the flow simulator will provide a mechanism for linking these models. We will develop case studies of coupling a groundwater model and geothermal reservoir model, to better represent the interplay between shallow groundwater processes and the deeper geothermal system.

5.5 Validation projects

We intend to develop a number of projects to validate the coupling of numerical-geophysical-chemical modelling codes. These validation projects will use the new flow simulator to better understand hydrothermal processes and multi-system relationships. The simplest involve transferring existing TOUGH2 reservoir models, including industry models of producing geothermal fields to the new flow simulator; developing the first New Zealand multisystem model to investigate hypothetical interactions between the systems; coupling chemistry and flow models; and coupling geophysics and flow models..

6. CONCLUSION

This research programme will develop next generation integrated geothermal modelling tools required to address modern demands of researchers, the geothermal industry and regulators. These tools include a new flow simulator, geophysical and geochemical codes, and the linkages between them. Coupling models from different disciplines will improve confidence in the predictive capabilities of the models. The research will provide improved approaches to model system connectivity, complex chemical interactions, rheology (e.g. geomechanics) and hydrology (e.g. multi-phase fracture flow, groundwater-geothermal interaction).

Examples of advances from the programme include:

- Improved numerics to enable fast, reliable reservoir simulations;
- Robustness of reservoir simulations, with a consistent approach to handle nonlinear features of the phase transitions and fluid properties;
- Incorporation of more complex chemistry into geothermal flow models to more accurately track conditions and predict fluid properties, whilst being computationally feasible;
- Coupled mechanical behaviour to the flow simulator to simulate thermo-hydro-mechanical effects on reservoir processes;
- Physically reasonable boundary conditions for large-scale models; and
- The ability to test different conceptual models of regional-scale flow processes that incorporate models of heat and mass flow, geophysics and geochemistry.

Improved modelling capabilities will allow for more robust predictions of resource characterisation, reservoir performance and improved field management. Our new modelling tools seek to serve the needs of the geothermal community for at least the next 15 years, will be designed to overcome inefficiencies, be more flexible, and better able to accommodate future needs.

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