An Integration Solution of Geomodelling Tools in a Geothermal Modelling Framework

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ABSTRACT

A new functionality in SKUA-GOCAD was developed, allowing it to create both the grid mesh and the deck file necessary for the Waiwera simulator. Through a combination of Python Scripts and JavaScript Macros, a user-friendly interface was created, simplifying the creation of Geothermal Simulation inputs. It is possible for any user to modify it on demand, making it an ideal candidate for integration in a modular geothermal modelling framework where flexibility is key. By construction, it can also be easily run in a batch mode, opening the door for sophisticated workflows like Assisted History Matching, Sensitivity Analysis, or Coupled Flow-Thermal-Geomechanical Simulations using thirdparty software. In addition to the advantages introduced by the new Macros, the existing advanced modelling functionality and the post-processing capabilities available in SKUA-GOCAD may also enhance the quality of the models produced.

1. INTRODUCTION

Geomodelling software dominant in the Oil and Gas industry have found successful applications in geothermal fields. Packages like Petrel (Sullera et al., 2021), Earth Vision (Siler et al., 2016) or SKUA-GOCAD (Hartline et al., 2015) all offer valuable features for geothermal exploration and production (Witter et al., 2018).

However, while these modeling tools are robust and have been well-established within their primary industry, they occasionally fall short in encapsulating functionality sought after by geoscientists in the geothermal industry. This results in experts often turning to a modular workflow using multiple specialized packages to perform specific distinct tasks, as discussed by O'Sullivan et al. (2023). This approach presents greater flexibility but requires seamless integration between the different components of the workflow.

Therefore, the challenge lies in integrating the robustness of traditional geomodelling tools with the niche specificity of geothermal software. Recent developments in SKUA-GOCAD have been focused on enhancing its scripting capabilities in both Python and JavaScript. The deeper customization offered extends to data exchange with open formats, making new synergies between separate systems possible.

This paper introduces a new workflow focusing on the integration of geocellular models constructed using standard modelling tools within a modular geothermal framework using geothermal simulators like TOUGH2 or Waiwera (Croucher et al., 2020), allowing geothermal modellers to tap into the strengths of workflows traditionally used by the Oil and Gas industry.

2. METHODOLOGY

2.1 Creation of Geological Model

Constructing a comprehensive geological model for simulation studies within the geothermal context necessitates integrating insights from diverse datasets and knowledge domains. At the forefront, the model encapsulates the geological characteristics, delineating upflow origins, recharge areas, resource dimensions, and factors regulating fluid movement, such as geological layers, structural elements, and zones of mineral alteration.

Prior to building the model, simulation studies require a clear initial problem statement, addressed by a preliminary analysis of the geophysical and geological data to define the major conceptual reservoir features. Data, relatively specific to geothermal reservoirs such as resistivity dataset (MT data) may be loaded and used as inputs for calibrating the geomodelling phase.

Various standard modelling tools are available to interpret major formation boundaries, represent them in structural models or in geocellular grids, and interpolate earth sample data to mimic the true subsurface distribution of the geological characteristics of the field.

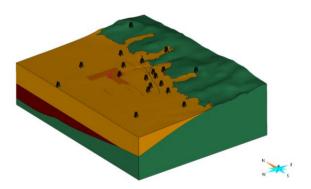


Figure 1: Geocellular model of the FORGE geothermal field (Courtesy of Utah)

Geothermal simulators that use a finite volume formulation typically require the grids to respect the orthogonality condition (Croucher et al., 2013). Traditional modelling tools and gridding algorithms usually do not have to follow that restriction, but it remains possible to generate compliant grids by creating single block models (i.e., no physical disconnection between the grid nodes) with vertical pillars. Meshes may still be customized with different element types, with varying mesh resolution, or with varying mesh orientation.

While the rest of the workflow presented here must be carried out in the SKUA-GOCAD software, this phase may be done in any package permitting connectivity with RESQML, Rescue or Eclipse ASCII/Binary formats.

2.2 Conversion of the Grid Geometry to a Mesh File

Once the grid geometry is deemed satisfactory, its mesh must be exported to a format supported by geothermal simulators. A direct export is available in SKUA-GOCAD for TOUGH2. For Waiwera, it must be in a format supported by the PETSc library's DMPLex unstructured mesh handling software. This includes the popular exodus or gmsh formats. This is done in two phases.

Firstly, the geocellular grid is exported in the widely-used Abaqus format. This step ensures a standardized representation of the 3D model, enabling a seamless transition between various software. If the model nodes and element centers are split into multiple files, they need to be unified under a single file following the Abaqus format. In the case of single block models, this is a straightforward step that can be carried out manually. Macro scripts are available to ensure the file consistency.

In the subsequent phase, the converted Abaqus format serves as the input to a simple Python script leveraging the meshio library. Meshio stands out for its capability to bridge numerous mesh formats, and in this context, it facilitates the transformation of the Abaqus format into either exodus or gmsh formats, depending on the user's preference.

2.3 Creation of a SKUA-GOCAD Macro

Macros, by definition, are a means of executing a series of commands as a single action, improving both efficiency and repeatability. In SKUA-GOCAD, a macro can be created as a new command constructed by streamlining existing commands, enriched with the capability to tap into a JavaScript API within the software data model.

A new command can be developed to create the JSON data file used as simulation input parameters for Waiwera. This was done in four steps:

- Definition of Variables: This delineates which elements of the script can be controlled by the user and what they are. This can be for example the grid Pressure-Temperature properties, the JSON file directory, the simulation results file name, the different rocks densities and permeabilities, or the simulation time stepping settings.
- Interface Designing: Once the variables are clearly earmarked, they can be arranged in an interface. It acts as the primary interaction point with the macro for the user, so intuitive structuring is essential.
 Variables falling under the same category (e.g.,

- rock parameters) have been grouped into tabs for easier navigation.
- Script Body Creation: a JSON object literal is created following Waiwera syntax. Care must be taken to define all mandatory keys or value pairs needed by the simulation process. If they are declared within the script body, they will remain constant each time the macro is executed. If they are defined as variables, they can be changed from the interface.
- Conversion to String: The data captured in the JSON object are converted into a string. This transformation facilitates a smooth and error-free writing to the text file, ensuring data integrity.

While it would be possible to write a macro flagging all the possible JSON keys as variables, in practice, it is easier to create several macros for generic cases. Typically, different equations of state used for the simulation will require different parameters. Building one command per set equation of state helps in alleviating the task of building complex variable inter-dependencies during the Interface Designing step. Thus, at present, it is critical to align the macro to the case it must export.

Figure 2 shows an interface example of a macro creating a JSON file with the parameters necessary for a simulation using a Water-Energy Equation of State.

The script utilized in this study is available upon request from the author. All SKUA-GOCAD users have the option to freely access and modify the script body at will with the embedded macro editing tools.

2.4 Post-Processing with Python Scripts

Simulation results written in an HDF5 format can be imported in SKUA-GOCAD using a Python script.

The current import script relies on ASCII conversion. Cell center coordinates and properties are transformed into points which can be upscaled to the initial simulation grid as time-dependent properties. Source term results can be written as a table and imported as well data.

3D Visualization tools, production plot, animations, scenario comparison and summary maps of time-dependent properties can then be leveraged to better understand the dynamic behavior of the reservoir.

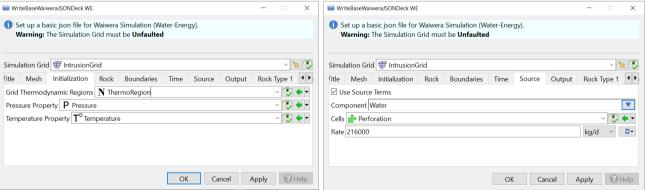


Figure 2: Macro command interface grouping different parameters into user-friendly tabs.

3. APPLICATION ON A SYNTHETIC CASE

The command has been successfully applied to initialize the simulation of a synthetic case presented in Figure 3 consisting of an upflow problem with two flat water-filled layers disrupted by a conical geological intrusion.

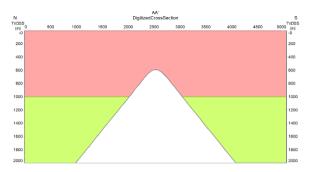


Figure 3: Initial Model Geometry

Without aiming to be exhaustive, the principal simulation parameters used to describe the model have been summarized in the table below.

Parameter	Region	Value
Model Extension	All	5 *5*2km
Grid Size	All	522801 cells
Time Step	All	~18 days
Equation of State	All	Water-Energy
Pressure	Тор	5000 kPa
	Bottom	15000 kPa
	Intrusion	20000 kPa
Temperature	Тор	20 °C
	Bottom	60 °C
	Intrusion	100 °C
Specific Heat	All	1000 kJ/(kg*K)
Permeability	Тор	1500 mD
	Bottom	1000 mD
	Intrusion	800 mD
Density	Тор	2500 kg/m^3
	Bottom	2800 kg/m^3
	Intrusion	3000 kg/m^3
Porosity	Тор	0.2
	Bottom	0.15
	Intrusion	0.01

The simulation converged after 45 min and 150 iterations (about 7 years). The results have been imported in SKUA-GOCAD for 3D visualization and are shown in Figure 4.

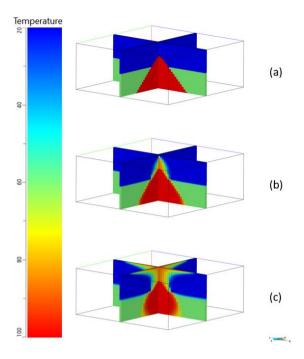


Figure 4: Field Temperature evolution at three different time step (a) t = 0 (b) t = 2 years (c) = 7 years.

Due to the much higher pressure and permeability contrast of the intrusion with the first layer rather than with the second layer, high temperature water flows vertically at the Top/Intrusion interface and permeates through the top layer. This remains the principal feature of the field throughout the rest of the simulation. At the last days of the simulation, the pressure drop caused by the vertical flow of the intrusion water causes the cooler water stored in the second layer to flow horizontally towards the intrusion rock. A downwards movement of the colder water in the top layer towards the bottom layer, due to gravity effects, can also be observed.

Alternative scenarios with a source term, a more realistic hydrostatic pressure profile and different rock parameters conditions could be quickly explored by simply editing the macro parameters. Sensitivity analysis results shown in Figure 5 highlighted the vertical permeability as the main parameter affecting the fluid flow in the current set-up.

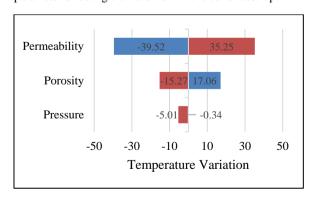


Figure 5: Tornado Chart of simulation parameters affecting the final temperature in the top horizon.

4. BENEFITS

4.1 Sophisticated Modelling Workflows

Geomodelling software basic modules offer by default the possibility to import geothermal data, visualize them in 3D, in maps or in graph views, and create conceptual models either manually or from subsurface objects. Figure 6 shows simultaneously in a 3D View microseismic data imported as time-dependent points, a DEM topography surface, Fracture azimuth logs as Rose Diagrams, and a geocellular property model, among other things.

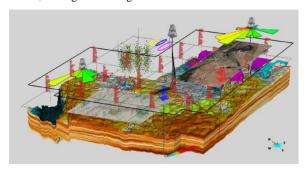


Figure 6: Multi-type data management and integration in SKUA-GOCAD.

While most of them have been designed to handle sedimentary geological environments, implicit-based advanced structural modelling options are available to recreate complex volcanic geological environments such as intrusions with multi-Z values or intricate fault and fracture network.

Property modelling tools help define initial conditions for the primary variables. Thermodynamic properties such as Pressure or Temperature can be created with a predefined gradient through scripting commands. Data Analysis procedures can extract trends (typically depth Gradients) from subsurface measurements, and Geostatistical algorithms like kriging may be used to interpolate them. Advanced Facies Modelling algorithms such as Multi-Point Statistics are available to realistically model distributions of rock types. Grid region arrays allow specific cells to be accessed during command operations based on various criteria, such as their location within a closed polygon, their association with specific facies, or their presence within distinct geological units. In the context of this paper, this is particularly useful when defining thermodynamic regions or constant rock regions variables (e.g., Specific Heat, Density, etc.).

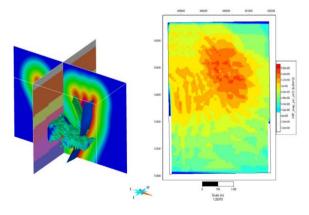


Figure 7: 3D play fairway analysis and heat-in-place per m^2 map of a geothermal field in SKUA-GOCAD.

Embedded commands specific to SKUA-GOCAD are dedicated to geothermal data and further extend the adaptability of the modeling pre-processing. Real case-studies examples include microseismicity analysis, export to the TOUGH2 simulator, or custom macros dedicated to the estimation of the Geothermal Potential in a 3D Grid with heat in place, theoretical capacity and technical potential. Figure 7 presents a 2D and 3D view of the command outputs.

Time-dependent visualization displays in 3D and in plot views may assist in post-processing tasks. Python libraries, similar to MatPlotLib, offer additional customization avenues within the SKUA-GOCAD environment.

4.2 Macro Command Advantages

One of the most obvious advantages offered by the macro functionality is its user-friendly interface streamlining the process of creating and updating deck files. This is a valuable time-saver for engineers and geoscientists who often need to iteratively customize simulation parameters to correctly initialize geothermal runs.

As highlighted in Section 4.1, grid "regions" can easily be modified and re-created at will in the JSON file. The easy and quick access of regions in the Macro facilitates the model description and gives a granular level of control on the set of cells used for flagging rock regions, faults settings, boundary conditions, or well locations.

Macros also come with embedded unit conversion tools for "Typed Quantity" variables, i.e., single numbers with an attached unit of measurement. Parameters such as Specific Heat, Density, Time Stamps, or Injection Rate can be automatically converted into arrays consistent with the Waiwera format. Such a feature removes the manual drudgery of unit conversion in the text file. Figure 8 shows the parameters available as inputs for the Rock Type section. Each physical quantity is automatically converted into the unit used by Waiwera.

Last, but not least, harnessing the JavaScript programming language for this macro ensures a robust generation of an error-free deck file, diminishing the need for tedious syntax QC procedures.



Figure 8: Macro tab for Rock Type parameters set up. More quantities can be added as variables if required.

4.3 Workflow Flexibility

O'Sullivan et al. (2023) consider the following criteria to be essential for a tool to be integrable in the modular approach the geothermal modelling framework follows:

- Outputs should be in an open format to facilitate exchange with other tools used in the framework.
- Scripting tools should be easy-to-use, re-usable and easy-to-modify.
- It should be flexible enough to adapt to various existing frameworks.

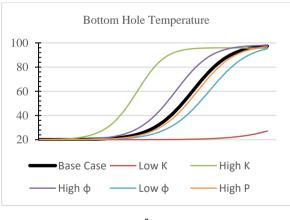
By construction, macros are open source, making them easy to modify and fit to given modelling set-ups. By combining SKUA-GOCAD import/export catalog and python scripts, data are freely transferred between software at any point of the workflow.

Although the software allows a large part of the workflow to be run in its internal environment (including postprocessing), it is possible to choose to use it for particular tasks and delegate others to more specialized tools if they offer a better option.

4.4 Uncertainty Analysis

Due to a general lack of data availability and/or reliability, subsurface uncertainties are typically fairly large in geothermal studies - to the point where making 3D Models at all is sometimes not considered worth the effort in some cases (Rattenbury et al., 2019). In all cases, the model uncertainty assessment and characterization remain a key challenge (Witter et al., 2018).

Macros allow automated runs with modifications on the parameters set as variables, making them ideal for sensitivity analysis and uncertainty quantification workflows. With the Macro player workflow, sets of JSON files can be automatically generated with different parameters.



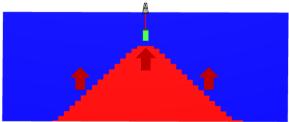


Figure 9: Comparison of Temperature evolution over time in different simulations with different parameters

A simplified version of the synthetic model introduced in Section 3 was created with a producing source term, as shown in Figure 9. Through the macro player workflow, uncertainty was introduced in several simulation parameters, and their impact on the resulting simulation was captured at the well level.

Macros can also be run in a batch mode with the parameter uncertainty defined externally to the software environment, meaning they may be integrated in any pre-set uncertainty optimization workflow. A prime example of this is their use in the Big Loop workflow (Fillacier et al, 2014; Abdallah et al., 2021). Using Aspen Tempest Enable as a workflow orchestrator, SKUA-GOCAD and Waiwera can be linked together in an Assisted History Matching process. This is done in 5 steps:

- Project Set-up: Configuration of SKUA-GOCAD JavaScript and Waiwera as workflow components.
- Uncertainty Parametrization: Definition of Macro Parameters uncertainty.
- Uncertainty Scoping: Running simulation runs sampling the full uncertainty field.
- Assisted History Matching Refinement: Make runs converge towards historical data by restraining uncertainty to relevant values.
- Prediction: Use History-Matched ensemble of runs to predict future field behavior.

Many interesting byproducts can be obtained from the approach presented in Figure 10: Probabilistic predictions, insights into field uncertainty, sensitivity analysis of static and dynamic parameters, evergreen models – to name a few.

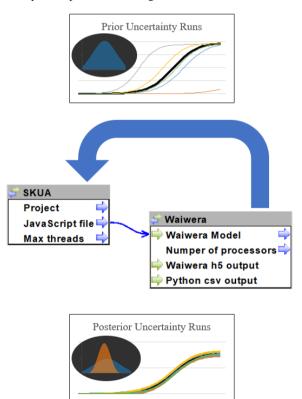


Figure 10: Initial set-up concept of the SKUA-Waiwera Big Loop with uncertainty definition in Tempest Enable.

4.5 Coupling to Geomechanical Simulations

Using the Abaqus format as the pivotal format for the mesh export opens the door to data exchange between geothermal simulation software like Waiwera or TOUGH2 to 3D geomechanical simulators like Abaqus or FLAC3D.

This compatibility facilitates a streamlined integration of thermal, hydraulic, and mechanical processes, allowing researchers and engineers to assess more comprehensively subsurface stress variations over time. Ultimately, a more rigorous understanding of the earth mechanics leads to more realistic estimations of failure risks and to safer and more efficient design of field development plans.

Typical cases of geomechanical simulations include subsidence analysis, fault reactivation risk assessment, and borehole stability studies. In the context of a geothermal field, coupling with a fluid and heat flow simulations helps to assess the additional impact of production on in-situ stresses and of the temperature effects on the rock mechanical parameters like Cohesion or Poisson's ratio.

Figure 11 shows a simple synthetic model (5*5*20 cells) simulated in an uncoupled simulation workflow using Waiwera. The geomechanical model was initialized with a hydrostatic pore pressure and a geostatic vertical stress. The fluid/heat simulation introduced a source term at the center of the model, causing a change of pore pressure and of temperature. These perturbations were imported into the geomechanical model, and a mechanical simulation was executed until equilibrium.

Relations between the temperature and the material properties were defined ad hoc. The temperature change had a minimal effect on the total stress field. However, the relative changes in the stress field showed the temperature change caused by the injection had effects akin to those

observed when drilling a well - albeit at a smaller scale of magnitude.

While the model run was simplistic, it proved to be enough to test the compatibility of the outputs generated by geothermal simulators like Waiwera or TOUGH2 with geomechanical simulators. Being derived from the same Abaqus grid, element centers share the same IDs, which make exports in ASCII straightforward. Geomechanical simulators also require certain properties to be written at the grid nodes, which could pose challenges to element-centered simulations. However, SKUA-GOCAD has useful standard exporters converting cell-center properties to corner-point properties if necessary and can act as the intermediary.

5. CONCLUSION

Using recent functionalities, a new workflow has been developed as a proof of concept to export SKUA-GOCAD results to a modular geothermal modelling framework.

Initial tests on synthetic models show promise in the ability of the tool to simplify the creation of input files for simulation. Whether this increased usability can lead to increased adoption will be decided by geothermal geoscientists after tests on real field cases.

This also opens the door to workflows traditionally used by the Oil and Gas industry that remains to be used by the geothermal industry. In particular, uncertainty optimization workflows have long been identified as a practice to implement, but tests with real historical production data are again necessary to assess the viability of the solution methodology.

Further developments of the software as a modelling solution for geothermal cases and of the macro as a solution within the geothermal modelling framework are still ongoing.

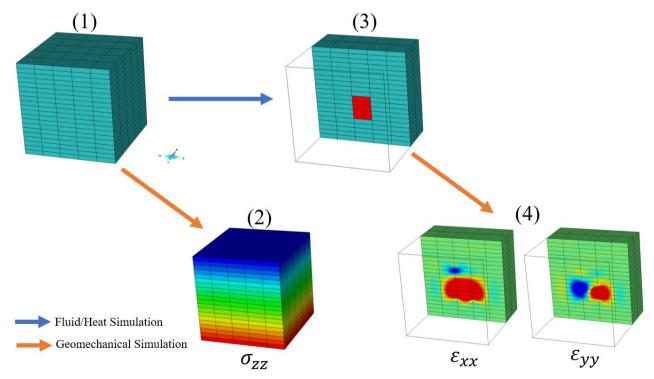


Figure 11: Uncoupled geothermal and geomechanical simulation. The model (1) is sent independently to a geomechanical initialization (2) and to Waiwera (3). New equilibrium is reached after perturbation of the mechanical model (4).

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