CREATING AN UNSTRUCTURED 2.5D TOUGH2 GRID GEOMETRY CONSTRAINED TO A GEOLOGICAL MODEL

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ABSTRACT

Flow simulation models aim to accurately forecast the flow through porous material, enabling subsurface teams to investigate a range of possible development scenarios. The simulation provides a spatially and temporally varying model of flow over a grid. Accuracy is dependent on how well the system is described by the governing equations of the flow model, how well the grid conforms to the geology of the system, the relative resolution of the grid compared to the spatial variations in flow over the system, and how well the connections between individual grid blocks adhere to the assumptions implicit in the numerical method. TOUGH2 allows for the simulation of coupled transport of water, vapour, non-condensable gas and heat in porous material (Pruess et al., 1999). Given its application to an appropriate system, related accuracy concerns include the generation, population and visualisation of a grid that aims to conform to the underlying geology of the system. Flow simulations are also computationally intensive, which practically limits the grid resolution to ensure the model converges in a timely manner.

We present tools and a workflow for creating and using an unstructured Voronoi 2.5D grid geometry in a TOUGH2 model in an attempt to better enable the reservoir simulation grid to conform to the geological units and features such as faults and well perforations within the system of interest. A Voronoi grid is used to increase the flexibility of the volume centroid locations while still adhering to the requirements of the TOUGH2's governing equations, namely, that the connections between adjacent volumes are orthonormal (Pruess et al., 1999, Croucher et al., 2013). The workflow allows for interactively creating and iteratively refining the grid geometry. Rock types from the geological model including fault rock types are evaluated on to the grid. The TOUGH2 model created is then exported to a Mulgraph geometry file and a TOUGH2 .DAT file.

1. INTRODUCTION

The workflow for simulating the coupled transport of water, vapour, non-condensable gas and heat in porous material with TOUGH2 includes generating a grid that conforms to both the underlying geology and regions of interest, appropriately populating this grid with material properties, defining the initial and boundary conditions of the system, and simulating the system. This gives a prediction of flows, pressures and temperatures through the system.

Poorly chosen material properties or initial conditions can result in inaccurate models, as can grids that do a poor job conforming to the underlying geology of the region. Grids that do not adhere to the geometrical assumptions that TOUGH2 is based on can also lead to slow convergence and inaccuracies in the simulation. As such, the simulation should be considered against any relevant measurements or other a priori information with the aim of assessing its validity. Any concerns about its accuracy should be used to inform updates to the grid geometry, material properties or initial conditions. For this reason, a streamlined workflow for grid generation, simulation and results visualisation is important.

In 2010 Leapfrog Geothermal 2.1 provided support for importing and exporting structured hexahedral TOUGH2 grids with the aim of streamlining and extending the TOUGH2 support in Leapfrog Geothermal to provide an interactive workflow solution for simulating and validating TOUGH2 simulations based on the geological information contained within a geological model. This allows modellers to more rapidly model and better understand the behaviour of a system based on its geology. In successive updates Leapfrog Geothermal added support for generating and populating hexahedral TOUGH2 grids based on the geological information contained within a geological model, and for visualising the time dependent simulation results. This functionality was completed in Leapfrog Geothermal 2.3 (Newson et al., 2012 and O'Sullivan et al., 2017)

This workflow relied on structured hexahedral grids, which are unable to conform to non-cartesian geological features. This limited the ability of modellers to use Leapfrog Geothermal to simulate complex geothermal systems with TOUGH2. The rest of this paper introduces a new workflow-based approach to generating 2.5D unstructured TOUGH2 grids in Leapfrog Geothermal 3.6 that are better able to adhere to typical geological features. The unstructured TOUGH2 grid and its generation are introduced in the 'Grid generation' section. The new adaptations to the workflow in Leapfrog Geothermal are introduced in 'Workflow' section. In the 'Discussion' section we consider the suitability of the new workflow before introducing some existing limitations and intended future work. We draw conclusions in the 'Conclusion' section.

2. GRID GENERATION

TOUGH2 simulations are based on the Finite Volume Method, in which the unknowns solved by the simulation are defined at the centres of the grid blocks. Practically, this means that grid blocks should be centred on features of interest such as faults and wells.

The mathematical formulation of the Finite Volume Method assumes that element centres are connected by a line that is perpendicular to the face connecting them (Berry et al., 2014). This is satisfied by cuboid and Voronoi grids with horizontal layering and fully unstructured Voronoi grids (Berry et al., 2014). We decided to use horizontally layered Voronoi grids as Voronoi grids can be constrained to follow non-cartesian grid aligned features. A horizontally layered approach was selected to allow for the resulting grid to be easily visualised for basic validation of its geometry and geological alignment by the user.

These layered Voronoi diagrams were generated from a Delaunay triangulation created using the GCAL[1] computing library, which implements Shewchuk's algorithm for producing conforming triangulations (Shewchuk, 2000). This algorithm allows constraint edges to be specified and for the maximum allowable triangle edge length to be set. Any triangle with an edge length greater than this resolution will be split. The algorithm also guarantees a minimum triangle angle of $\sin^{-1}(1/\sqrt{8}) = 20.7\text{deg}$ in triangles that do not have any constraint edges (Shewchuk, 2000).

As discussed in the workflow section, the triangulation is constrained to conform to the features of interest within the geological model, such as faults and wells, and any other features selected by the user. Voronoi diagrams are the dual of a Delaunay tessellation (Alliez et al., 2010), and the conversion from a Delaunay triangulation to a Voronoi diagram ensures that these features of interest are centroid aligned in the resulting Voronoi diagram. The only ambiguity in this conversion exists around the border of the Delaunay tessellation where there are no more triangles. A set of Voronoi cells are created around the border that extend to perpendicularly across the border to ensure that Voronoi grid extents encompass the geological model.

Support for independent simplification of each feature is provided by individually pre-processing the constraint feature to reduce the number of points defining the constraint before these are introduced to the Delaunay triangulation algorithm as edge constraints. The local refinement around each feature is achieved by adding constraint points near features that the user wishes to be surrounded by a higher resolution grid.

3. WORKFLOW

The unstructured gridding workflow introduced in Leapfrog Geothermal 3.6 provides a solution for Voronoi grid generation, population and visualisation of the results in Leapfrog. The workflow includes support for importing and exporting TOUGH2 grid geometry information using the Mulgraph format (O'Sullivan et. Al, 1995) and TOUGH2 .DAT files (Pruess, 1999). These formats are widely supported allowing the user to simulate the system with their preferred version of TOUGH2.

The workflow enables the user to generate the grid based on a geological model and any other features or input data they choose to include. The grid is then populated with rock types based on the geology of the geological model. As with other objects created in Leapfrog, a change in the user's selection leads to a dynamic update of the grid. Similarly, the algorithm allows for the user to dynamically specify which individual features are included as constraints in the grid. The user can review the effect of feature inclusion and refinement on grid size and quality.

[1] CGAL the computational geometry algorithms library: https://www.cgal.org/

3.1 Creating a TOUGH2 unstructured grid

In the new workflow, the creation of a TOUGH2 model is based on an existing geological model that the geologist has created, combined with available data such as wells, faults and geophysical data.

The geological modelling process involves several steps including importing well and other required data, then creating a basic geological model of lithological units, refining its boundary and defining a fault system. The fault system partitions the geological model into sub-units known as fault blocks as shown in Figure 1.

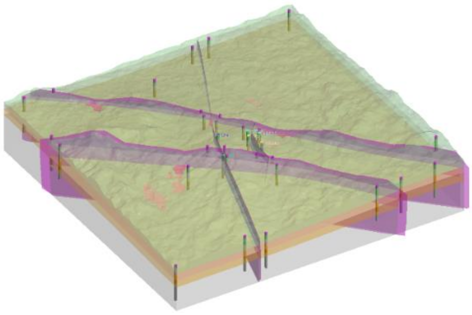

Figure 1: Geological model with faults

Each TOUGH2 unstructured grid must be associated with a geological model. The grid geometry is controlled by a number of factors, some of which can be inherited from the geological model, including:

- boundary
- default block size
- features such as wells, faults, points and polylines
- simplification and tolerance settings

All grids must have a boundary and default block size as shown in Figure 2. Features may then be added later based on the modeller's interpretation and regions of interest.

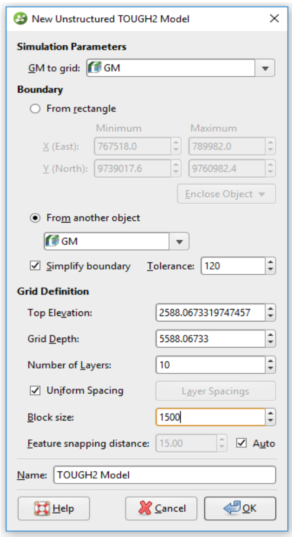

Figure 2: Creating a new TOUGH2 model

The **Block size** setting determines the basic size of the grid blocks, although the size will vary according to features applied to the grid and the **Feature snapping distance**. The effects of the **Feature snapping distance** do not become apparent until features have been added to the grid. A grid generated from the geological model shown in Figure 1 with the geological model's faults and wells is shown in Figure 3.

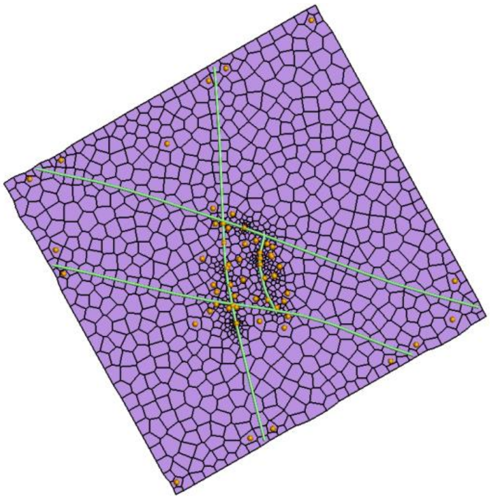

Figure 3: 2D unstructured Voronoi grid with wells and faults shown

Typically, the boundary for the TOUGH2 grid will either be rectangular or the boundary of the associated geological model. The complexity of the boundary directly impacts the local resolution of the Voronoi cells surrounding the boundary. A boundary that is defined by a curved polyline or by points that are closely spaced relative to the grid block size will result in Voronoi cells that have an increased resolution around the boundary. If this undesirable, we have implemented a **Simplify boundary** option which reduces the number of points along the boundary. This will reduce the total number of grid blocks generated and increase the relative size of the Voronoi cells around the boundary. Reducing the **Tolerance** value increases the number of points along the boundary. The two settings together let you define a basic boundary with blocks that are roughly uniform in size, set by the value of **Block size**.

Once the grid has been created, features can be added. These constrain the tessellation so that Voronoi cells spanning these features are centroid aligned with these features. Each feature has an associated **Tolerance** and **Snapping distance** that controls the simplification of that feature much like the boundary.

The resulting grid is a 2.5D unstructured grid, by which we mean it is unstructured in x, y and layered in z. The thickness of the layers can be edited. Grid blocks in a layer will have the same thickness except where they have been clipped by the top surface of the parent geological model.

Once the TOUGH2 model with its initial grid has been created, the hierarchy of the model is shown in the project tree, as shown in Figure 4. This highlights the dependencies within the model, e.g. the 2D unstructured grid is dependent on the boundary, the geological model and features such as wells and faults. Any changes to these dependent data or models will trigger a rebuild of the grid geometry.

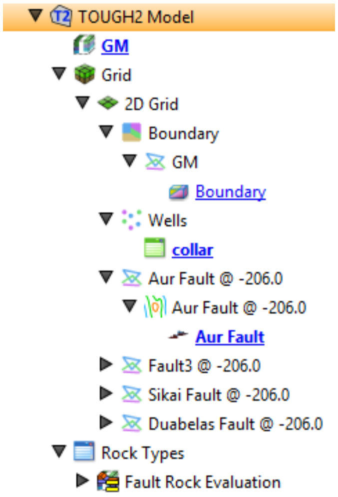

Figure 4: TOUGH2 model hierarchy showing objects used in gridding

3.2 Iteratively updating the grid

Once the initial grid has been generated it can be iteratively updated as new data is collected and the modeller's understanding of the geothermal system evolves. This is a process by which the user improves how well the grid conforms to the underlying geology to a point where further improvements do not improve the accuracy / granularity of the model beyond the base requirements.

The main method for controlling the gridding is to use features which constrain the centroid locations of the grid blocks. Typical features include the wells and faults associated with the geological model. However, we can also add more generic objects such as user defined points and polylines.

3.2.1 Wells

When the grid is created, wells from the geological model are added to the grid as features. Individual wells can be turned on or off as control points for the gridding, as shown in Figure 5. Well control points are defined either as the mid-point of well screens (perforations) if these are available, or the top well location (x, y). These control points each define the centroid locations of a grid cell. As with all features, a snapping distance can be set by the user to combine closely spaced well control points.

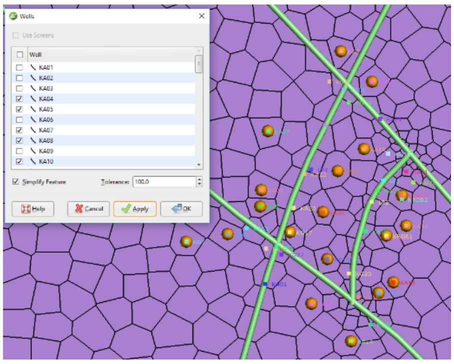

Figure 5: Removing individual wells as features to control the gridding

3.2.2 Faults

When the geological model used to define the model is faulted, the model's faults will be included in the TOUGH2 grid as features. Rather than the full fault surface, points along a polyline evaluated from the surface at a user specified depth as 2.5D grids cannot faithfully mesh off-vertical surfaces. These are used as the control points, as shown in Figure 6.

Currently, the user can control the depth at which the surface is evaluated to create a polyline (Figure 7) but does not have direct control over the positioning and spacing of the control points along the polyline. However, like other features the user can control the relative refinement around the fault. This will lead to smaller centroid aligned elements along the fault.

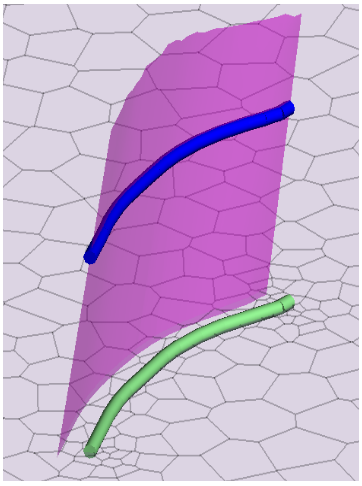

Figure 6: Polyline from a fault evaluated at a specified depth is used to control the gridding

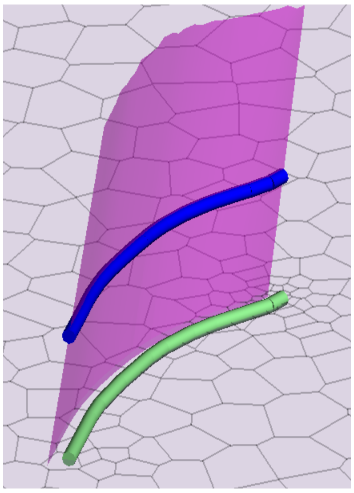

Figure 7: Re-evaluating the fault at a lower depth changes the gridding

3.2.3 Gridding to other features

Other generic data objects such as user defined points or polylines can also be added as features by the user. One example is to define two sets of gridded points, one at a higher density spacing and one with sparser spacing towards the outer regions of the grid. An example is shown in Figure 8. Note that there are some gridding artifacts at the boundary.

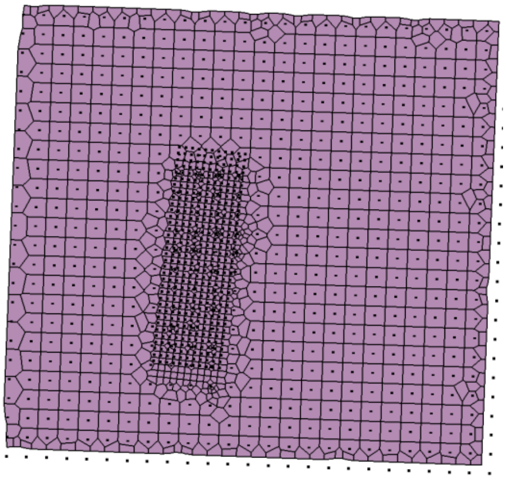

Figure 8: Gridding with points as features

3.2.4 Boundary

The boundary of the grid may often be a simple rectangular shape. However, the user can specify an alternative boundary, for example, using a polyline or the extents of another data object or model (Figures 9 and 10). As previously noted, the gridding algorithm is sensitive to both the shape and the number of points on this boundary.

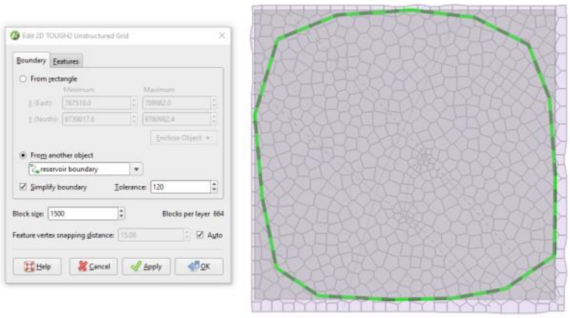

Figure 9: User defined boundary for the gridding

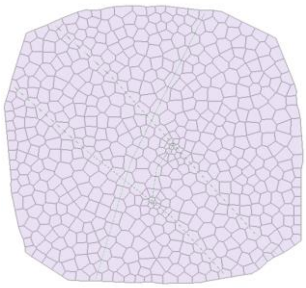

Figure 10: 2D unstructured grid with user defined boundary

3.2.5 Evaluation of rock types on to the grid

As the geometry is updated, the rock type evaluation is also updated. This evaluation is based on both the lithological units and the faults in the associated geological model, as shown in Figure 11. The specification of fault rock types was added to the structured hexahedral TOUGH2 workflow in Leapfrog Geothermal 3.5 and updated to support the unstructured TOUGH2 grid in Leapfrog Geothermal 3.6.

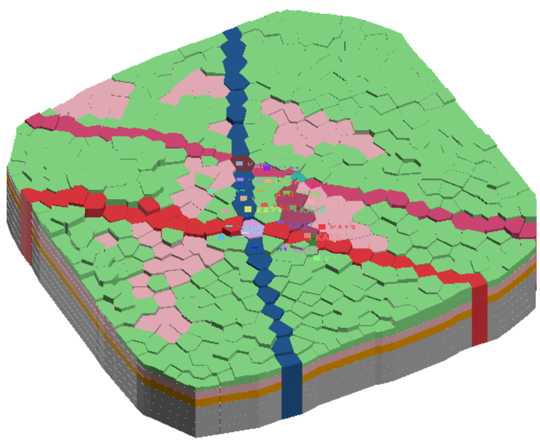

Figure 11: TOUGH2 unstructured grid with rock types

4. DISCUSSION

The unstructured TOUGH2 workflow described in this paper should allow for the generation of grids that better conform to the underlying geology and thus allow for either improved accuracy in the flow simulation or the same level of accuracy for a coarser grid. The workflow aims to allow this information to be more readily incorporated so that the grid on which the simulation is based can be viewed and updated more holistically and rapidly based on new data and an evolving understanding of the geothermal system.

4.1 File formats

There is no standard grid geometry format for TOUGH2 which does not use an explicit geometry. Instead the grid is defined by a set of grid blocks with volumes and connectivity between those blocks. Typical TOUGH2 models have tens of thousands of grid blocks. Defining the volumes and inter-block connections for 10,000 grid blocks is non-trivial. The most common-sense solution is to use some sort of underlying grid geometry.

Two openly available (and openly defined) gridding formats have grown in use by the geologists and engineers using TOUGH2 to become de-facto standards. These are:

- The Mulgraph/Mulgrid geometry (O'Sullivan and Bullivant, 1995) and the PyTOUGH software library (Croucher, 2011) were developed by the Geothermal Institute at Auckland University
- The AMESH format and software developed by LBNL

Initial support was added for the Mulgraph format due to its greater relevance in the New Zealand context.

4.2 Grid quality

The unstructured grid generation approach described in this paper supports the inclusion of features as constraints and the introduction of local refinement around the features. As mentioned in the Workflow section the constraints can be simplified or snapped together. When constraints with closely spaced points are added this leads to locally refined Voronoi cells as shown in Figure 12. This may or may not be desirable and careful consideration should be given by the modeller to the appropriate level of simplification and the appropriate snapping distance applied to constraint features and/or the grid boundary.

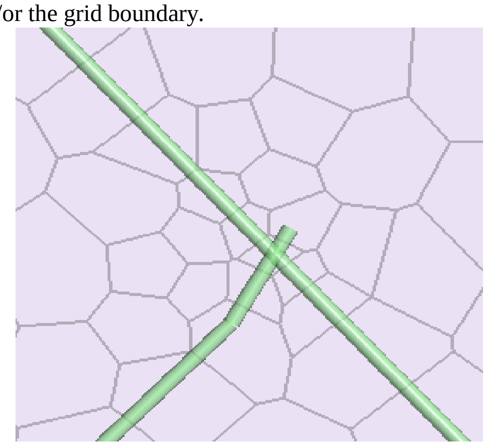

Figure 12: Proliferation of small grid blocks where two line constraints meet (in this case, faults)

As mentioned in the grid generation section, the Voronoi diagram is generated from a Delaunay tessellation, which is guaranteed to have orthonormal connections between adjacent cells. This satisfied the base requirement of the Finite Volume Method upon which TOUGH2 is based.
The geometric quality of the Voronoi cells still needs to be considered as Voronoi cells with large variations in the face area with adjacent cells, as shown in Figure 13, can lead to both a reduction in the solution accuracy and numerical instabilities in the simulation (Croucher et al., 2013).

Figure 13: Voronoi grid cells with large aspect ratios

4.3 Grid optimisation

Based on the grid quality considerations introduced in the previous section, we have investigated the primary causes of reductions in grid quality, and an industry standard approach to improving the quality of Delaunay tessellations and their duals. Grid constraints appear to be the primary cause of poor quality grid elements, for example, acutely angled constraints and closely spaced constraints relative to the overall resolution of the grid as highlighted in the Delaunay tessellations shown in Figure 14 and 15.

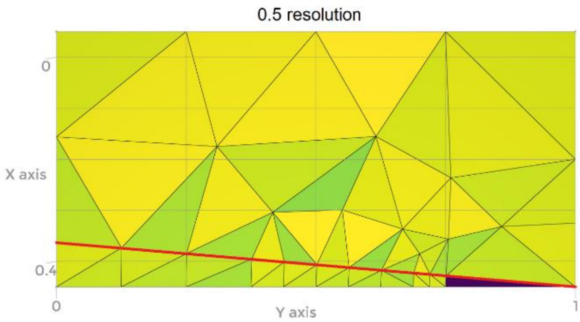

Figure 14: An acutely angled constraint and the resulting poor-quality grid element. Triangles coloured by aspect ratio.

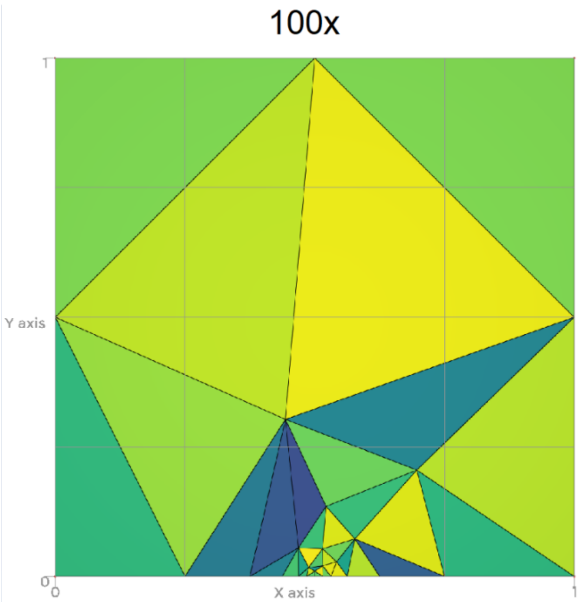

Figure 15: A point constraint which is 100x closer to the boundary than the overall mesh resolution. Again, triangles coloured by aspect ratio.

There are established routines for optimising the quality of grids. Mesh optimisation is the adjustment of its nodes or connectivity to improve it according to some quality metric. The Lloyd optimisation routine (Lloyd, 1982), which is available from CGAL 3.1 acts to adjust the triangle node locations to minimise the global energy. As such it does not change the mesh connectivity. Figure 16 considers the effect of both the number of Lloyd iterations applied, and also the level of distortion in the initial mesh on the quality of the final mesh. This shows the minimum, maximum and median quality of two meshes after 0-100 optimisation iterations. Both meshes have a constraint point placed near the border. One has a resolution 2x this spacing with no obvious localised distortion, while the other has a resolution 100x the spacing and does exhibit substantial localised distortion.

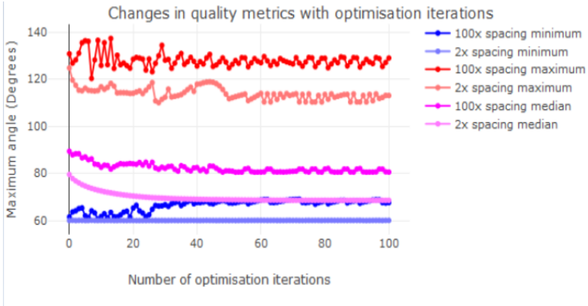

Figure 16: The effect of optimisation on a poor-quality mesh (100x spacing) and a relatively normal quality mesh (2x spacing).

These plots show that the quality of the worst triangle, and to a lesser extent the median value, varies substantially between optimisation iterations (both improving and worsening) in the mesh with a resolution 100x the constraint spacing. In contrast, the mesh with a resolution 2x the constraint spacing has much less volatility in the worst-case value and a steadily improving median value. This suggests that the modeller should make careful consideration of the impact of feature constraints on the quality of the Delaunay tessellation (and resulting Voronoi diagram).

5 FUTURE WORK

The workflow presented in this paper aims to allow TOUGH2 modellers to more effectively and accurately model geothermal systems. It is the authors' belief that there are several areas of development that could make the Leapfrog Geothermal unstructured TOUGH2 support more versatile. These include:

- Support for the AMESH TOUGH2 geometry format, so that more TOUGH2 modellers can access the Leapfrog unstructured TOUGH2 workflow.
- Display basic Voronoi cell quality metrics, so that users can better assess the impact of adding and simplifying feature constraints on grid quality.
- Allow modellers to specify the snapping distance and the level of simplification applied to the discretised control points extracted from faults.

6. CONCLUSION

We present a workflow aimed at facilitating the generation of a grid that better conforms to the underlying geology by generating Voronoi grids based on geological features of interest. This should improve the accuracy of the simulation allowing for a high accuracy or a fast simulation run time for the same accuracy.

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