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Into the Noddyverse: A massive data store of 3D geological models for Machine Learning & inversion applications

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18 **Abstract**

19

20 Unlike some other well-known challenges such as facial recognition, where Machine Learning and Inversion algorithms are
21 widely developed, the geosciences suffer from a lack of large, labelled ~~dataset~~data sets that can be used to validate or train
22 robust Machine Learning and inversion schemes. Publicly available 3D geological models are far too restricted in both number
23 and the range of geological scenarios to serve these purposes. With reference to inverting geophysical data this problem is
24 further exacerbated as in most cases real geophysical observations result from unknown 3D geology, and synthetic test
25 ~~dataset~~data sets are often not particularly geological, nor geologically diverse. To overcome these limitations, we have used
26 the Noddy modelling platform to generate one million models, which represent the first publicly accessible massive training
27 set for 3D geology and resulting gravity and magnetic ~~dataset~~data sets. This model suite can be used to train Machine Learning
28 systems, and to provide comprehensive test suites for geophysical inversion. We describe the methodology for producing the
29 model suite, and discuss the opportunities such a model suit affords, as well as its limitations, and how we can grow and access
30 this resource.
31

1 Introduction

Although it has become the focus of intense research activity in recent times, with more papers published in the five years prior to 2018 than all years before that combined, Machine Learning (ML) techniques applied to geoscience problems dates back to the middle of the last century (see Van der Baan and Jutten, 2000, and Dramsch, 2020, for reviews). ML ~~methods are being applied~~ applications relate to a whole range of geological and geophysical problems, but many of these studies face common challenges due to the nature of geoscientific ~~dataset~~ data sets. Karpatne et al. (2017) summarise the principal challenges as follows:

- i. Objects with Amorphous Boundaries- ~~the~~ The form, structure and patterns of geoscience objects are much more complex than those found in discrete spaces that ML algorithms typically deal with, consisting of both changes in topology and dimensionality of geoscience objects with time.
- ii. Spatio-temporal Structure- Since almost every geoscience phenomenon occurs in the realm of space and time, we need to consider evolution of systems in order to understand the current state.
- iii. High Dimensionality- The Earth system is incredibly complex, with a huge number of potential variables, which may all impact each other, and thus many of which may have to be considered simultaneously.
- iv. Heterogeneity in Space and Time- Geoscience processes are extremely variable in space and time, resulting in heterogeneous ~~dataset~~ data sets in terms of both sparse and clustered data. In addition, the primary evidence for a process may be erased by subsequent processes.
- v. Interest in Rare Phenomena- In a number of geoscience problems, we are interested in studying objects, processes, and events that occur infrequently in space and time, such as ore deposit formation and earthquakes.
- vi. Multi-resolution Data- Geoscience data-sets are often available via different sources and at varying spatial and temporal resolutions.
- vii. Noise, Incompleteness, and Uncertainty in Data- Many geoscience data-sets are plagued with noise and missing values. In addition, we often have to deal with observational biases during data collection and interpretation.
- viii. Small sample size- The number of samples in geoscience data-sets is often limited in both space and time, which of course is accentuated by their high dimensionality, (iii) and our interest in rare phenomena (v). In the case examined in this study, ~~the total number of there are few~~ publicly available 3D geological models, ~~s probably numbers less than 10,000000~~, and they are stored in a wide variety of formats, rendering comparison difficult.
- ix. Paucity of Ground Truth- Even though many geoscience applications involve large amounts of data, geoscience problems often lack labelled samples with ground truth.

In this study we specifically focus on six of these challenges by providing a database of one million 3D geological models and resulting gravity and magnetic fields. We address the *Spatio-temporal Structure* of the system by using a kinematic modelling engine that converts a sequence of deformation events into a 3D geological model. We address *High Dimensionality* by generating a very large database of possible ~~outeomes~~ 3D geological models. This represents a fundamental point of difference from many ML targets such as those studying consumer preference or movie rating or facial recognition. Although of course every human face is different, with few exceptions we share the same number of features (eyes, ears, noses), and these features' size and relative positions only varies within small bounds. The number, geometry, composition and relative position of features in the subsurface has very wide bounds and this represents a major hurdle to the application of ML to characterising 3D geology. This challenge is shared by more traditional geophysical inversion approaches (Li and Oldenburg, 1998).

71 We address issues related to *Multi-resolution Data* by providing a ‘controlled’ [datasetdata set](#), at the same resolution, it offers
72 possibilities to address multi-resolution issues, by subsampling or upscaling.

73 We address *Noise, Incompleteness, and Uncertainty in Data* by providing synthetic data, we have noise and uncertainty free
74 data, or at least under control, and complete spatial coverage over the simulation domain. The models we provide can easily
75 have a structured or unstructured noise added to them and they can be subsampled to reproduce incomplete [datasetdata sets](#).

76 We address *Small sample size* by generating one million models, which is certainly not enough to thoroughly explore the high-
77 dimensional model space; however, it illustrates the feasibility of producing large suites of models in the near-future. Modern
78 ML training sets for popular subjects such as the human face may contain tens of millions of examples (Kollias and Zafeiriou,
79 2019). A search of the Kaggle database of training [datasetdata sets](#) (<https://kaggle.com>, which contains over 63,000 distinct
80 [datasetdata sets](#) at the time of writing) only had 151 with geoscience in the keywords, and only seismic catalogues featured as
81 geophysical data. Similarly, only 59 [datasetdata sets](#) contained 3D data, and none were related to the geosciences.

82 Finally, we address the spatial and temporal *Paucity of Ground Truth* by publishing over one million models for which the
83 full 3D lithological and petrophysical distribution is provided in a labelled form for comparison with resulting gravity and
84 magnetic fields. This challenge is also faced by geophysical inversion methods. 3D geological models built using sufficient
85 data to reduce uncertainty arguably exist, but leaving aside a strict definition of uncertainty, well-constrained 3D geological
86 models are primarily restricted to restricted areas of significant economic interest, specifically sedimentary basins and mineral
87 deposits, which only represent a sub-set of possible geological scenarios. A number of studies have built simple or complex
88 synthetic models as a way to overcome these problems by providing fully defined test cases for testing processing, imaging
89 and inversion algorithms (Versteeg, 1994; Lu et al., 2011; Salem et al., 2014; Shragge et al., 2019a and b). Whilst these
90 provide valuable insights, the efforts required to build these test cases preclude the construction of large numbers of
91 significantly different models. It is easy enough to vary petrophysical properties with fixed volumes, however varying the
92 geometry, and, in particular, the topology is time consuming.

93 [Implicit geological modelling is based on the calculation of scalar fields that can be iso-surfaced to retrieve stratigraphy and](#)
94 [structure, as opposed to earlier methods that were CAD-like or based on interpolation of datapoints.](#) Recent advances in
95 implicit modelling allow extensive geology model suites to be generated by perturbing the data inputs to the model (Caumon,
96 2010; Cherpeau et al., 2010; Jessell et al., 2010, Wellmann et al., 2010a & b; Wellmann, and Regenauer-Lieb, 2012; Lindsay
97 et al., 2012; Lindsay et al., 2013a and b; Lindsay et al., 2014; Wellmann et al., 2014; Wellmann et al., 2017, Pakyuz-Charrier
98 et al., 2018 a & b, 2019) as part of studies that characterised 3D model uncertainty, however since they use a single model as
99 the starting point for the stochastic simulations, these works do not provide a broad exploration of the range of geological
100 geometries and relationships found in nature. Work on the automating of modelling workflows may allow us to explore the
101 model uncertainty space more efficiently (Jessell et al., 2020).

102 In this study, we have created a massive open-access resource consisting of one million three-dimensional geological models
103 using the Noddy modelling package (Jessell, 1981; Jessell & Valenta, 1996). These are provided as the input file that defines
104 the kinematics, together with the resulting voxel model and gravity and magnetic forward- modelled response. The models
105 are classified by the sequence of their deformation histories, thus addressing a temporal *Paucity of Ground Truth*. This resource
106 is provided to anyone who would like to train a ML algorithm to understand 3D geology and the resulting potential field
107 response, or to anyone wishing to test the robustness of their geophysical inversion techniques. Guo et al. (2021) used the
108 same modelling engine to produce more than three million models of a more restricted range of parameters to train a ML
109 Convolutional Neural Network system to estimate 3D geometries from magnetic images. In this study we aim to provide a
110 much broader range of possible geological scenarios as the starting point for a more general exploration of the geological
111 model space.

Field Code Changed

112 The Noddy software has been used in the past for a range of studies due to its ease in producing ‘reasonable-looking’
113 geological models with a low design or computational cost. A precursor to this study used a hundred or so manually specified
114 models as a way of training geologists in the interpretation of regional geophysical ~~dataset~~~~data sets~~ by providing a range of
115 3D geological models and their geophysical responses (Jessell, 2002). Similarly, Clark et al. (2004) developed a suite of ore
116 deposit models and their potential-field responses. The automation of model generation using Noddy was first explored using
117 a Genetic Algorithm approach to modifying parameters as a way of inverting for potential-field geophysical data, specifically
118 gravity and magnetics (Farrell et al., 1996). Wellmann et al. (2016) developed a modern Python interface to Noddy to allow
119 stochastic variations of the input parameters to be analysed in a Bayesian framework. Finally Thiele et al. (2016 a,b) used this
120 ability to investigate the sensitivity of variations in spatial and temporal relationships as a function of variations in input
121 parameters.

122
123 In this study we draw upon the ease of generating stochastic model suites to build a publicly accessible database of one million
124 3D geological models and their gravity and magnetic responses.

125 2. Model construction

126 The Noddy package (Jessell, 1981; Jessell & Valenta 1996) provides a simple framework for building generic 3D geological
127 models and calculating the resulting gravity and magnetics responses for a given set of petrophysical properties. The 3D model
128 is defined by superimposing user-defined kinematic events that represent idealised geological events, namely base stratigraphy
129 (STRAT), folds (FOLD), faults (FAULT), unconformities (UNC), dykes (DYKE), plugs (PLUG), shear zones (SHEAR-
130 ZONE) and tilts (TILT), which, can be superimposed in any order, except for STRAT, which can only occur once and has to
131 be the first event. 3D geological models are calculated by ~~taking~~ the current x,y,z position of a point and unravelling the
132 kinematics (using idealised displacement equations) until we get back to the time when the infinitesimal volume of rock was
133 formed, whether defined by the initial stratigraphy, or the time of formation of a stratigraphy above an unconformity, or an
134 intrusive event. In this study, we only use the resulting voxel representation of the 3D geological models, however it is possible
135 to produce iso-surface representations of the pre-deformation location of points in an implicit scheme. We have used this tool
136 as it is rapid, taking under 15s to generate 200x200x200 voxel models with both geological and geophysical representations
137 combined using an Intel(R) Xeon(R) Gold 6254 CPU @ 3.10GHz processor, and produces ‘geologically plausible’ models
138 that may occur in nature. Given that the final 3D model depends on the user’s choice of a geological history, Noddy can be
139 thought of as a kinematic, semantic, implicit modelling scheme.

140 As opposed to Wellmann et al. ((2016),), Thiele et al. (2016) and Guo et al. (2021), who used a ~~p~~Python wrapper to generate
141 stochastic model suites, in this study we have modified the C code itself to simplify use by third parties, although the
142 philosophy of model generation is an extension of, but very similar to, these earlier studies. The most significant difference is
143 that we have added petrophysical variations by randomly selecting from a set of stratigraphic groups, see next section.

144 Figure 1 shows one example model set for a STRAT-TILT-DYKE-UNC-FOLD history, consisting of a 3D visualisation
145 looking from the NE of the voxel model, with some units rendered transparent for clarity, the top surface of the model an EW
146 section at the northern face of the model looking from the south, a NS section on the western face of the model looking from
147 the east, and the resulting gravity and magnetic fields.

148 3. Choice of Parameters

149 In this section we describe the choices and range of values for the parameters that we have allowed to vary for our one million
150 model suite. We recognise there are other unused modes of deformation that Noddy allows that have been ignored. The
151 selection of these parameters is based on assessing the range of parameter values that will produce suites of models that we
152 believe will help and not hinder addressing the challenges cited in the introduction to this work. For example, we limited the
153 size of the plugs so that a single plug could not replace the geology of the entire volume of interest. In the discussion, we refer
154 to additional event parameters that could be activated in future studies. We limited the study to five deformation events,
155 starting with an initial horizontal stratigraphy which is always followed by tilting of the geology. The following three events
156 are drawn randomly and independently from the event list comprised of folds, faults, unconformities, dykes, plugs, shear
157 zones and tilts. The likelihood of folds, faults and shear-zones are double the other events as we found, [based on a qualitative](#)
158 [assessment](#), that they had a bigger impact of changing the overall 3D geology, and hence we wished to sample more of these
159 events. This means we can have $7^3=343$ distinct deformation histories, although the specific parameters for each event can
160 also vary, so the actual dimensionality of the system is much higher. For clarification, the one million models are not the result
161 of a combinatorial approach, but of one million independent draws using a Monte Carlo sampling of the model space. [Whilst](#)
162 [a combinatorial approach may in theory explore the parameter space more uniformly, the sequence of 5 deformation events is](#)
163 [so non-linear that it was reasoned that a pure MC approach would serve our purposes.](#)

164 The initial stratigraphy as well as new, above-unconformity stratigraphies, are defined to randomly have between two and five
165 units to keep the systems relatively simple, but this could of course be increased if desired. The lithology of each unit in a
166 stratigraphy is chosen to be coherent with the specific event and other units in the same sequence, so that we do not, for
167 example, mix high-grade metamorphic lithologies and un-metamorphosed mudstones in the same stratigraphic series (Table
168 2) nor do we assign the petrophysical properties of a sandstone to an intrusive plug. Once a lithology is chosen, the density
169 and magnetic susceptibility is randomly sampled from a table defining the Gaussian distribution of properties (linear for
170 density, log-linear for magnetic susceptibility) for that rock type. In the case of densities this may result in occasional negative
171 values, however since the gravity field is only sensitive to density contrasts this does not invalidate the calculation. Some rock
172 types have bimodal petrophysical properties to reflect real-world empirical observations, so we draw from a Gaussian mixture
173 in these cases. The petrophysical data is drawn from aggregated statistics (mean and standard deviation of one or two peaks)
174 of the approximately 13,500 sample British Columbia petrophysical database (Geoscience BC, 2008).

175 The parameters which can be varied for each type of event, together with the range of these parameters, is shown in Table 1.
176 These parameters can be grouped in the shape, position, scale and orientation of the events, and for a five-stage deformation
177 history require the random selection of a minimum of 23 parameters for a STRAT-TILT- TILT - TILT - TILT model up to 69
178 parameters for a STRAT-TILT-UNC-UNC-UNC model where each stratigraphy has five units. Apart from the petrophysical
179 parameters, all other parameters are randomly sampled from a uniform distribution.

180 Any subset of the geology can be calculated for any sub-volume of an infinite Cartesian space using Noddy, but we limit
181 ourselves to a 4x4x4 km volume of interest in this study. Similarly, although the geology within this volume can be calculated
182 at an arbitrary resolution, we have chosen to sample it using equant 20 m voxels as this is well below the typical resolved
183 measurement scale for these types of data when collected in the field.

184
185 Geophysical forward models were calculated using a Fourier Domain formulation using reflective padding to minimise (but
186 not remove) boundary effects. The forward gravity and magnetic field calculations assume a flat top surface with a 100 m
187 sensor elevation above this surface, and the Earth's magnetic field with vertical inclination, zero declination and an intensity
188 of 50,000 nano-tesla.

4. Results

The 7^3 possible event histories produce 343 possible sequences which averages to 2915 models per sequence. Given the imposed bias towards folds, faults and shear zones, different event sequences were more or less likely to be found in the 1M model suite, and the high-probability event sequences (e.g. FAULT-SHEAR ZONE-FOLD) produced 8245 models and while the low-probability event sequences (e.g. UNC-TILT-PLUG) produced only 905 models. The different combinations produced, with plateaux in the number of models calculated giving event sequence frequencies at around 1000, 2000, 4000 and 8000 depending on the number (0,1,2,3 respectively) of events in the sequence. Together these form a “Noddyverse” of one million 3D geological models and their gravity and magnetic responses. Figure 2 shows an arbitrarily selected suite of 100 models as a 10x10 grid showing the top surface and two sections of the model as in Fig 1, together with the resulting gravity and magnetic fields, to show the variability of the results.

5. Applications

The same logic of using millions of Noddy models was first applied by generating a massive 3D model training set and used to invert real-world magnetic data (Guo et al. 2021). That study used a model suite consisting of only FOLD, FAULT and TILT events, and only one of each to predict 3D geology using a Convolutional Neural Network. This approach corresponds to a use case where prior geological knowledge as to the local geological history has been used to limit the model search space, and formal expert elicitation could provide an important pre-cursor step to support the generation of sensible and tractable problems (citations). In addition to the CNN training demonstrated by Guo et al. (2021), we can envisage three broad categories of studies that could build upon the 3D model database we present here:

- 1) **Studies into the uniqueness of 3D models relative to geological event histories.** The principal question here is whether any form of clustering-classification of the patterns seen in of the geophysical fields, and perhaps the including map of the surface, can be used to recover the event sequence or event parameters. Feature extraction techniques are well-known for supporting image classification and clustering, so using the same principles, can we identify unique clusters of forward models from the Noddyverse, and do these clusters then correspond to distinct histories? Likewise, can we train a classifier with extracted features from the forward models of the gravity and magnetic responses which can then successfully identify models with similar or the same histories. Three broad aspects need to be considered here: (1) the feature extraction method; (2) choice of pre-processing methods for dimensionality reduction (Self Organising Maps, Principal Component Analysis, Kernel-Principal Component Analysis, t-distributed Stochastic Neighbor Embedding etc.) and (3) the clustering (k-means, hierarchical methods, DBSCAN /OPTICS) or classification methods (random forests, support vector machines, linear classifiers).

A study of geophysical image variability using a simple 2D correlation or maximal information coefficient between pairs of images of different histories would be illuminating. Do we have images which are the same (or at least very similar and within the noise tolerance of the geophysical fields) to each other, but belong to very different histories? If these exist, the ambiguity of the histories can be examined, and we then know where we would expect poor performance from ML techniques which rely on easily discriminated images. The systems of equations characterising geophysical inverse problems often have a non-unique solution. In ML research, if we only use magnetic data or gravity data for inversion, we will be troubled by the non-uniqueness of the solution. However, because we have both gravity data and magnetic data, we can extract features from multi-source heterogeneous data at the same time, and then classify or regress after feature fusion. This could greatly reduce the influence of the non-unique solution. Having a large set of models will allow clustering of models accordingly to their geophysical response and identifying

subsets of geological models that are geophysically equivalent and cannot be distinguished using geophysical data. The analysis of diversity of such subsets of models will give an estimate of the severity of non-uniqueness and allow the derivation of posterior statistical indicators conditioned by geological plausibility.

- 2) **Comparison between ~~and~~-training schemes of ML systems.** We see potential applications of deep learning techniques (e.g., Convolutional Neural Network and Generative Adversarial Networks) where the series of models we propose may also be complemented by other ~~dataset~~data sets. In this broad topic we would seek to understand which ML techniques are suitable and effective in mapping geophysical data back to the geology or geological parameters. We can see potential for investigating which techniques minimise the amount of data necessary to get a good constraint, i.e., the model structures that most successfully capture geological expert knowledge? This could be framed as an open challenge to allow different groups to use their preferred approach to the inversion problem.
- 3) **Validation of the robustness of geophysical inversion schemes.** As previously mentioned, one of the limitations to validating geophysical inversion schemes is the small number of test models available, with the resulting danger that the inversion parameters are tuned to the specifics of the test model, rather than being generally applicable. The Noddyverse model suite allows researchers to ~~trial-test~~ their inversions against a wide range of scenarios. It will also allow the examination of the validity and generality of hypotheses at the foundation of several integration and joint inversion procedures. One well-known example is the underlying assumption that the underlying models vary spatially in some coherent fashion (Haber and Oldenburg, 1997; Gallardo and Meju, 2003; Giraud et al., 2021, Ogarko et al., 2021). The analysis of geophysically equivalent models will also enable us to estimate how significantly joint inversion or interpretation can reduce the non-uniqueness of the solution, with the potential to identify families of geological scenarios more suited to joint inversion than others. It is obvious that some 3D geological models will be geologically more complex than others, and that some could be used for the benchmark of deterministic geophysical inversion of gravity and magnetic data, but also of other geophysical techniques relying on wave phenomena. The dataset presented here contains all required ingredients for the training of ML surrogate models for general applications similar in spirit to Athens and Caers (2021), who train a surrogate ML model on realizations already sampled by Monte Carlo simulation and show that it is very advantageous computationally. While the work they present is performed in 2D, it is safe to assume that this may hold in 3D, which enables another avenue for further use of the Noddyverse.

6. Discussion

In this study we have produced a ML training ~~dataset~~data set that attempts to address four recognised limitations of applying ML to geoscientific ~~dataset~~data sets, namely *Spatio-temporal Structure, High Dimensionality, Small sample size, and Paucity of Ground Truth, Multi-resolution Data & Noise, Incompleteness, and Uncertainty in Data*. Contrary to ~~the current trend~~usual practice, the work for the generation of a comprehensive suite of geological models did not depend on the ~~appropriate manual training-labelling of a neural network data~~. We relied solely on geoscientific theory and principles while remaining computationally efficient. While realistic-looking suites of geological models have been generated using Generative Adversarial Networks (Zhang et al., 2019), these ~~are generally represent a limited to a several thousands of samples, within a limited-range of geological scenarios, and the lack of extensive training samples.~~

6.1 Spatiotemporal Structure

Noddy is by design a Spatio-temporal modelling engine that uses a geological history to generate a model. Simple variations in the ordering of three events following two fixed events (STRAT & TILT), even with fixed parameters quickly demonstrates

the important of relative time ordering to final model geometry (Fig. 3). While Noddy is limited to simple sequential events, nature presents geological processes to be coeval (such as syn-depositional faulting) or partially overlapping resulting in complex spatiotemporal relationships (Thiele et al., 2016a). Nonetheless, re-ordering only sequential events still produces a vast array of plausible geometries, and indicates the enormity of the model space, and the necessity of efficient methods to explore them.

6.2 High Dimensionality

We have limited ourselves to five deformation events in this study, and no more than five units in any one stratigraphy. These decisions were based on an idea to “keep it simple” whilst simultaneously allowing a great variety of models to be built. We recognise that these are somewhat arbitrary choices. We could have true randomly complex 3D histories, leading to models with, for example, nine phases of folding, however the utility of over-complicating the system is not clear, and would rarely or ever be discernible in natural systems. Similarly, we limited the parameter ranges of each deformation event, again on the basis that the ranges chosen made models that are more interesting. For example, there did not seem much interest in having folds with very large wavelengths or very low amplitudes, as they are equivalent to small translations of the geology and would translate in the geophysical measurements into a regional trend that is often approximated and removed from the measurements.

Noddy is capable of predicting continuous variations in petrophysical properties, including variably deformed magnetic remanence vectors and anisotropy of susceptibility, or densities that vary away from structures to simulate alteration patterns, however we decided to limit this study to simple litho-controlled petrophysics, whilst recognising the interest of studying more complex discrete-continuous systems. The indexed models could also be reused with different, simpler petrophysical variations, such as keeping constant values for each rock type. Each model comes with the history file used to generate the model and this provides the full label for that model, so that if additional information, such as the number of units in a series is considered to be important, this can be easily extracted from the file.

6.3 Small sample size

The total number of models sounds impressive, however once we divide that number by the 343 different event sequences, we are left with between 905 and 8245 models per sequence, which whilst still large is by no means exhaustive. There is no fundamental problem with building 10 or 100 million models, and if this is found to be necessary to provide useful ML training ~~dataset~~[data sets](#) we can certainly do so at the expense of an increased compute time: these models were built in around a week on a computer using 20 processor cores. We can also follow try to apply a metric, such as model topology, to analyse how well sampled the model space is. Thiele et al. (2016b) analysed the topology of stochastically generated Noddy models and found that after 100 models for small perturbations around a starting model, the number of new topologies dropped off rapidly. In our case we are not making small perturbations, so we could expect to require more models before the rate of production of new topologies decays, and topology is only one possible metric for comparing models.

6.4 Paucity of Ground Truth

The primary goal of this study was to build a large ~~dataset~~[data set](#) to provide a wide range of possible models for use in training ML systems and to test more traditional geophysical inversion systems. The models here, whilst simpler than the large test models mentioned earlier, represent to our knowledge the largest suite of 3D geological models with resulting potential field data and tectonic history, which has its own utility. This usage applies equally well to classical geophysical inversion codes, which have traditionally been tested on only a handful of synthetic models prior to being applied to real-world data, for which there is no ground truth available.

306 6.5 Expert Elicitation

307 To use this suite of models as the starting point for inversion of real-world ~~dataset~~data sets (as has been pioneered by Guo et
308 al., 2021) we can envisage the introduction of expert elicitation methods to meaningfully constrain the model output space
309 while acknowledging our inherent uncertainty regarding the model input space. As a probabilistic encoder of expert
310 knowledge, formal elicitation procedures (O’Hagan, 2006) have contributed greatly to physical domain sciences where
311 complex models are essential to our understanding of the underlying processes. From climatology/meteorology/oceanography
312 (Kennedy, 2008), to geology and geostatistics (Walker, 2014, and Lark et al., 2015), to hydrodynamics and engineering
313 (Astfalck et al., 2018, and Astfalck et al., 2019), the central role of expert elicitation is being increasingly recognised. The
314 complexity and parameterizations of geophysical models, and the expert knowledge that resides within the geophysical
315 community, suggests this domain should be no different. It is worth noting that the choice of parameter bounds used to define
316 the 1 million model suite in this article is itself an informal expression of expert elicitation.

317 Once a targeted structure is reasonably well characterised, the approach taken by Guo et al. 2021 or thoroughly exploring a
318 narrow search space becomes possible. Unfortunately, in many parts of the world there is no outcrop available, due to tens to
319 hundreds of metres of cover. In this scenario, it makes sense to start with a broader search for possible 3D models that may
320 match the observed gravity or magnetic response, given their inherent ambiguity. We can imagine a hierarchical approach
321 where a subset of the 1M models is identified as possible causative structures, and then these are accepted or rejected based
322 on the geologist’s prior knowledge, and the accepted models are then used as the basis for a focussed parameter exploration.
323 In addition within the 1M model suite, it is currently possible to filter the models based on event ordering, and with minor
324 modifications to the code, it would be possible to filter on any parameter, such as fold wavelength.
325

326 6.6 Extending to the model suite

327 In the future we may need a better representation of the “real world” 3D model space, specifically to:

- 328 • Include more parameters from Noddy, especially for parameters such as fold profile variation, alteration near structures
329 to allow petrophysical variation within units. This would help to address the Karpatne et al. (2017) challenge of *Objects*
330 *with Amorphous Boundaries*. These are capabilities that exist within Noddy but are not used in this study.
- 331 • Allow more events to increase the range of outcomes. We arbitrarily restricted ourselves to two ~~started~~starting events
332 (STRAT and TILT) followed by three randomly chosen events, and an extension to the model suite could consider any
333 number of events in the sequence.
- 334 • Include magnetic remanence and anisotropy effects. At present we only model scalar magnetic susceptibility but the
335 Noddy modelling engine can calculate variable remanence and anisotropic magnetic susceptibility as well.
- 336 • Allow linked deformation events. At the moment every event is independently defined, however we could allow
337 parallel fault sets or dyke swarms, situations which commonly occur in nature.
- 338 • Predict different types of geophysical fields. For example, the SimPEG package (Cockett et al., 2015) could easily be
339 linked to this system to predict electrical fields (Cockett et al. 2015).
- 340 • Model larger volumes as large, or deep features cannot currently be modelled due to the 4 km model dimensions.
- 341 • Build more models. We in no way believe we have explored the range of possible models in the present model suite,
342 and if we ~~start in~~include more events, or more complex event definitions, we will certainly have to generate many more
343 models, perhaps orders of magnitude more, in order to provide robust training suites and inversion scenarios.

- Add noise to the petrophysical models and/or the resulting geophysical responses. This would help to address the Karpatne et al. (2017) challenge of *Noise, Incompleteness, and Uncertainty in Data*. *Incompleteness* can be addressed by removing parts of the geophysical data and does not require new models to be built. Similarly, the challenge of *Multi-resolution Data- Geoscience* could be addressed by subsampling parts or all of existing geophysical outputs.
- Include topographic effects. In this study, we have ignored the effect of topography on the models, although again this could be included in the future, as it is supported by Noddy.

We also need to be clear that a model built in Noddy is not capable of predicting all geological settings, as all Noddy models are plausible geology, but not all plausible geology can be modelled by Noddy. To improve this situation, we would need to improve the modelling engine itself. Similarly, the logic of trying to predict geology from geophysical ~~dataset~~data sets in this study is only partially fulfilled: the geometry comes from geological events sequence, but identical geometries can be produced by different event sequences.

7. Conclusions

This study represents our first steps in producing geologically reasonable training sets for ML and geophysical inversion applications. We have used Noddy to generate a very large, open-access 1M model, set of 3D geology and resulting gravity and magnetic models as a ML training sets. These training sets can also be used as test cases for gravity and/or magnetic inversions. The work presented here may be a first step to overcoming some of the fundamental limitations of applying these techniques to natural geoscientific ~~dataset~~data sets.

8. Acknowledgements

We acknowledge the support from the ARC-funded Loop: Enabling Stochastic 3D Geological Modelling consortia (LP170100985), DECRA (DE190100431) and Data Analytics for Resources and Environment ITTC (IC190100031). The work has been supported by the Mineral Exploration Cooperative Research Centre whose activities are funded by the Australian Government's Cooperative Research Centre Programme. This is MinEx CRC Document 2021/52. This work was further supported by the ARC Data Analytics for Resources and Environments ITTC (IC190100031). ~~We would like to thank AARNET for supporting this work by hosting the 500GB model suite at CloudStor.~~ Jiateng Guo received financial support from the National Natural Science Foundation of China (41671404). We would like to thank AARNET for supporting this work by hosting the 500GB model suite at CloudStor.

9. Code and Data availability

A doi (<https://zenodo.org/record/4589883>) provides access GitHub repository which contains the following elements (Jessell, 2021):

1. The source code (C language) for the version of noddy adapted to producing random models.
2. A readme.md file with a link to the windows version of the Noddy software, plus a link to 343 tar files, one for each event history ordering of the model suite.

- 378 3. A Jupyter Notebook (python code) for sampling from and unpacking the models.
- 379 4. A link in the same readme.md file to the equivalent *mybinder.org* version of the notebook so that no code
- 380 installation is required to sample from and view the model suite:
- 381 <https://mybinder.org/v2/gh/Loop3D/noddyverse/HEAD?filepath=noddyverse-remote-files-1M.ipynb>

382 All codes and data are released under the MIT licence.

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383 10. Author Contribution

384 Mark Jessell wrote the original and modified noddy software, ran the experiments and wrote the python software for

385 visualising the models. Jiateng Guo and Yunqiang Li were in-volved in conceptualisation and manuscript preparation. Mark

386 Lindsay, Jérémie Giraud and Guillaume Pirot were involved in the conceptualisation, as well as in co-writing the introduction

387 and discussions sections of the paper. Vitaliy Ogarko, Richard Scalzo and Ed Cripps were involved in developing and co-

388 writing the introductions and discussion sections of the manuscript.

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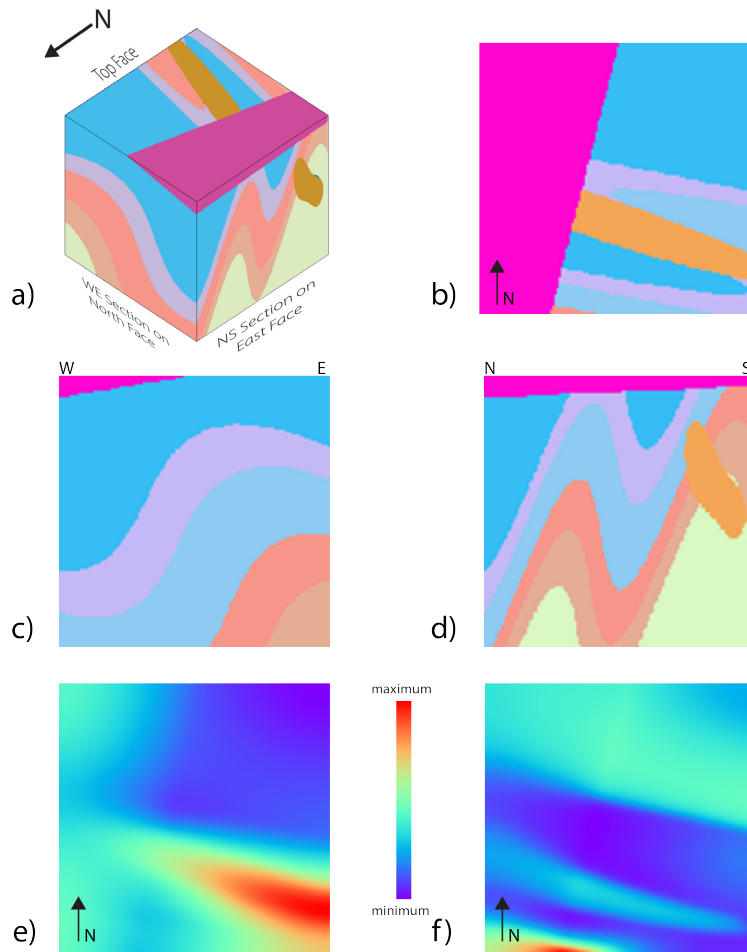


Figure 1. Example model set for a STRAT-TILT-DYKE-UNC-FOLD sequence showing a) 3D visualisation looking from the ~~NE~~ NW of the voxel model, b) the top surface of the model, c) an EW section at the northern face of the model looking from the south, d) a NS section on the western face of the model looking from the west, and the resulting e) gravity and f) magnetic fields. Geophysical images are all normalized to model max-min values.

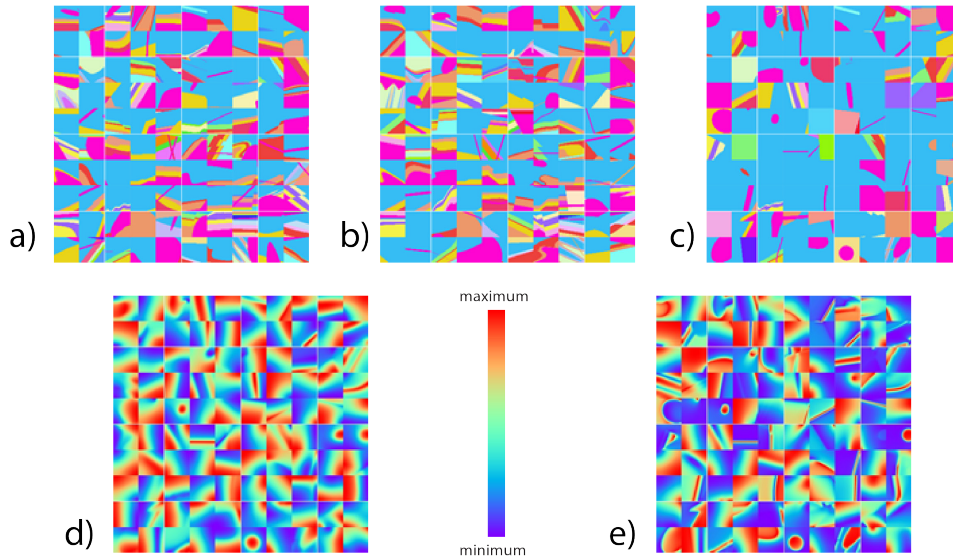
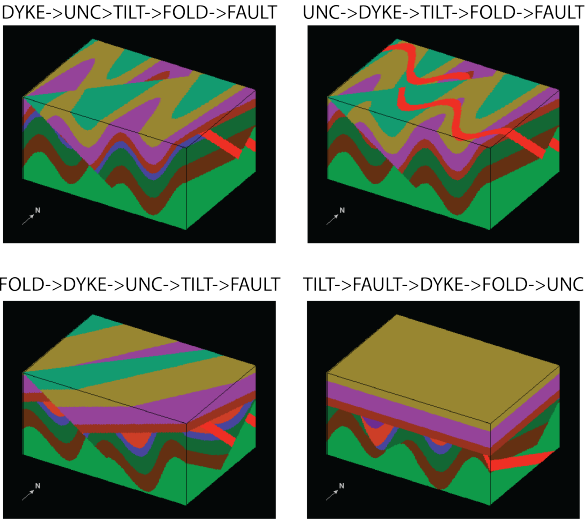


Figure 2. Example models for 100 randomly selected models drawn from the 1M model suite showing a) the top surface of the model, b) an EW section at the northern face of the model looking from the south, c) a NS section on the western face of the model looking from the west, and the resulting d) gravity and e) magnetic fields. Geophysical images are all normalized to model max-min values.

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518 **Figure 3. Four possible 3D geological models with the same base stratigraphy (STRAT) followed by five events using four of the**
519 **possible different event ordering sequences.**

Event type	Parameter 1	Parameter 2	Parameter 3	Parameter 4	Parameter 5	Parameter 6	Min/Max number of parameters
Base Stratigraphy	Number of units. Range: 2-5	unit n thickness: 50-1000 m	Density of each unit: depends on lithology of unit n	Magnetic susceptibility of each unit: depends on lithology of unit n			5/12
Fold	Wavelength : 1,000-11,000 m	Amplitude : 200 - 5,000 m	Azimuth : 0-360 degrees	Inclination : 0-90 degrees	Phase : 0-4000 m	Along axis amplitude decay : 500-9,500 m	6/6
Fault	Position of 1 point on fault: x,y,z 2000-4000 m	Displacement : 0-2000 m	Azimuth : 0-360 degrees	Inclination : 0-90 degrees	Pitch of displacement : 0-90 degrees		7/7
Unconformity	Position of 1 point on Unconformity: x=2000-3000m y=2000-4000m z=3000-4000 m	Number of units above unconformity: 2-5	Azimuth : 0-360 degrees	Inclination : 0-90 degrees	Density of each unit: depends on lithology of unit n	Magnetic susceptibility of each unit: depends on lithology of unit n	10/17
Dyke	Position of 1 point on fault: x=0-4000 m y=0-4000 m z=0-4000 m	Azimuth : 0-360 degrees	Inclination : 0-90 degrees	Width of Dyke : 100-400 m	Density : depends on lithology	Magnetic susceptibility : depends on lithology	8/8
Plug	Shape : Cylindrical, Conic, Parabolic, Ellipsoidal	Position of centre of plug: x=1000-4000m y=1000-4000m z=1000-4000m	Size of plug: parameter varies with shape	Density : depends on lithology	Magnetic susceptibility : depends on lithology		7/9
Tilt	Position of 1 point on rotation axis: x=2000-3000m y=2000-4000m z=3000-4000 m	Azimuth : 0-360 degrees	Inclination : 0-90 degrees	Rotation : -90-90 degrees			6/6
Shear zone	Position of 1 point on fault: x,y,z 2000-4000 m	Displacement : 0-2000 m	Azimuth : 0-360 degrees	Inclination : 0-90 degrees	Pitch of displacement : 0-90 degrees	Width of Shear Zone : 100-2000 m	8/8

Table 1. Free parameters with their allowable ranges for each event.

Lithology	Lithology Class	Genetic Class	Mean Density g.cm-3	Standard Deviation Density	Mean Log Susceptibility (cgs)	Standard Deviation Log Susceptibility	Susceptibility Bimodality Flag
Felsic Dyke Sill	Dyke	Intrusive	2.612593	0.090526329	-3.693262	1.50094258	1
Mafic Dyke Sill	Dyke	Intrusive	2.793914	0.015759637	-2.119223	0.85376583	0
Granite	Plug	Intrusive	2.691577	0.094589692	-2.455842	0.86575449	1
Peridotite	Plug	Intrusive	2.851076	0.154478049	-1.158807	0.4390425	0
Porphyry	Plug	Intrusive	2.840024	0.128971814	-2.613833	0.99194475	1
Pyxenite Hbndite	Plug	Intrusive	3.194379	0.253322535	-1.946615	1.03641373	0
Gabbro	Plug	Intrusive	3.004335	0.159718751	-2.124022	0.82126305	1
Diorite	Plug	Intrusive	2.851608	0.134656746	-2.088111	0.81829275	1
Syenite	Plug	Intrusive	2.685824	0.115078068	-2.461453	0.91295395	1
Amphibolite	Met strat	Metamorphic	2.875933	0.142164171	-2.69082	0.90733619	1
Gneiss	Met strat	Metamorphic	2.701191	0.073583537	-3.18094	0.95259725	1
Marble	Met strat	Metamorphic	2.871775	0.532997473	-3.671996	1.25374051	0
Meta Carbonate	Met strat	Metamorphic	2.738965	0.036720136	-3.117868	0.82945531	0
Meta Felsic	Met strat	Metamorphic	2.782584	0.301451931	-3.55755	0.65748564	1
Meta Intermediate	Met strat	Metamorphic	2.894892	0.265153614	-3.673276	0.26107008	0
Meta Mafic	Met strat	Metamorphic	2.814461	0.096381942	-3.250044	0.62513286	0
Meta Sediment	Met strat	Metamorphic	2.982992	0.49439556	-3.402807	0.89505466	1
Meta Ultramafic	Met strat	Metamorphic	2.843941	0.138208079	-2.166206	0.76543947	0
Schist	Met strat	Metamorphic	2.81978	0.109752597	-3.18525	0.69584686	0
Andesite	Met strat	Volcanic	2.721189	0.091639014	-2.15826	0.71678329	0
Basalt	Met strat	Volcanic	2.79269	0.155153198	-2.155728	0.64718503	0
Dacite	Met strat	Volcanic	2.62127	0.129131224	-2.562422	0.8166926	0
Ign V Breccia	Met strat	Volcanic	2.910459	0.101746428	-2.706956	0.73116944	0
Rhyolite	Met strat	Volcanic	2.630833	0.071233818	-3.046728	0.78711701	0
Tuff Lapillistone	Met strat	Volcanic	2.64447	0.110173772	-2.878701	0.86889142	0
V Breccia	Met strat	Volcanic	2.771579	0.167796457	-2.524945	0.90943985	0
V Conglomerate	Met strat	Volcanic	2.755267	0.10388303	-2.304483	1.00991116	0
V Sandstone	Met strat	Volcanic	2.779715	0.101133121	-2.903361	0.82701019	0
V Siltstone	Met strat	Volcanic	2.859347	0.102741619	-2.769054	0.87771183	0
Conglomerate	Strat	Sedimentary	2.618695	0.116158268	-3.31026	0.9740717	0
Limestone	Strat	Sedimentary	2.713912	0.147683486	-4.256256	0.87772406	0
Pelite	Strat	Sedimentary	2.698554	0.021464631	-3.369295	0.5295974	1
Phyllite	Strat	Sedimentary	2.739177	0.173374383	-3.696455	0.73955588	0
Sandstone	Strat	Sedimentary	2.622672	0.107003083	-3.452758	0.64521521	0
Greywacke	Strat	Sedimentary	2.861463	0.16024622	-3.841047	1.14724626	1

524 Table 2. Simplified petrophysical values derived from British Columbia database (Geoscience BC, 2008). Values are randomly
525 sampled from Gaussian distributions defined by mean and standard deviation of density and log magnetic susceptibility. For
526 lithologies with bimodal magnetic susceptibilities (flag=1), mixed sampling is based on offsetting the means by +/-0.75 orders of
527 magnitude, which approximates the variations seen in nature.