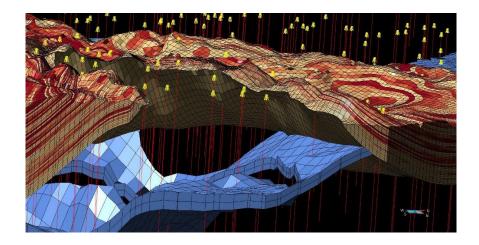


# Implicit Geological Modelling: a new approach to 3D volumetric national-scale geological models

Hydrogeology Programme Internal Report OR/19/004



### BRITISH GEOLOGICAL SURVEY

HYDROGEOLOGY PROGRAMME INTERNAL REPORT OR/19/004

# Implicit Geological Modelling: a new approach to 3D volumetric national-scale geological models

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Contributor/editor

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## Summary

This report provides information on implicit geological modelling and a possible application in the construction of national-scale (in the UK context) volumetric geological models. The stratigraphy of the UK is reviewed in the context of unconformity-bound stratigraphic sequences and how these can be applied in the modelling process. A range of input datasets are outlined with discussion on how these can be used and where gaps exist in available information. Model outputs are discussed highlighting the new opportunities offered by 3D stratigraphic grids. Some of the advantages and disadvantages of implicit modelling are discussed.

## 1 Introduction

Geological models are three-dimensional (3D) computer visualisations of the subsurface that attempt to show the spatial distribution of rock (or sediment) types and their related properties, their bounding surfaces, and associated structural discontinuities such as faults. The primary aim of most geological modelling is to allow an estimation of a selected geological property at any point within a subsurface volume of interest. This information might be required in different forms and for different reasons by, for example, a hydrogeologist, an actuary, a petroleum geologist, or a civil engineer. Predictive geological models are required because in most cases the observed or known distribution of geological properties in the subsurface (such as those obtained from boreholes) represents an extremely small sample of the overall volume of interest. Where appropriately attributed with geomechanical and flow-related properties such as permeability geological models also form the basis for dynamic simulations of the subsurface (Ringrose and Bentley, 2015).

A prerequisite for geological models that will allow the estimation of a property at any point in subsurface space is that they provide coverage of the entire volume of interest. This simple statement conceals what is in reality a challenging task because it involves the creation of gridded volumes that must replicate the often complex stratigraphical and structural geometries found in the subsurface. Moreover, rock volumes do not remain static over time but are often modified by later deformation: such post-depositional changes often need to be removed from gridded volumes to ensure the correct relationships of properties related to original depositional processes (Mallet, 2004). The requirement is thus not only for irregular, deformed 3D grids but for those that are capable of structural restoration.

The aim of this report is to outline a method of geological modelling that, although relatively new, has had a major transformative effect on the creation of 3D gridded volumetric representations of the subsurface. The method is termed implicit geological modelling and is a volumetric, semiautomated geological modelling approach that differs considerably from conventional explicit methods (Calcagno et al., 2008; Wellmann and Caumon, 2018). Implicit modelling methods have been successfully deployed in the British Geological Survey (BGS) over a number of years on targeted studies within individual basins (Newell et al., 2016; Newell et al., 2015b). This report describes exploratory attempts to use implicit modelling to generate a full volume 3D geological model at a national (Great Britain) scale. Given the stratigraphical and structural complexity of Great Britain this is not a trivial task. At present, national-scale geological models of GB are largely restricted to fence diagrams consisting of intersecting cross-sections (Waters et al., 2015).

The report provides some background to implicit modelling, considers how the stratigraphy of GB might be broken up into genetic units suitable for implicit modelling, discusses a range of available input data and outlines some of the derived products. The report represents the product of a number of years of research across a number of BGS supported projects including Permo-Triassic Reservoirs and Storage (PETReS), Hydrogeology 3D, Chalk3D, National Geological Model (NGM) and Hydro-JULES. Geological modelling is a broad and dynamic area of research. Geological models are invariably built for a highly specific purpose using the most appropriate software that is available. Information contained within this report in no way represents a BGS strategy for geological modelling or BGS endorsement of particular commercial software products.

## 2 The need for a new geomodelling approach

### 2.1 THE PROBLEMS OF EXPLICIT GEOLOGICAL MODELLING

Geological modelling is in essence a linear process that converts primitive objects with XYZ coordinates such as points into volumetric 3D grids (Figure 1). This transformation typically proceeds through two intermediate stages represented by polyline and surface objects (triangulated irregular networks or 2D grids). In terms of mapping these features to real-world geological objects, points might include stratigraphic picks in a borehole, while polylines could represent the linkage of these points in a cross-section, a picked horizon on a seismic reflection profile, a structure contour, or the intersection of a geological horizon with the topography (crop line on a map). Surfaces might represent a stratigraphic horizon or a fault.

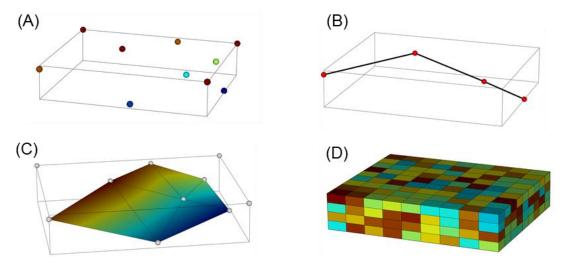


Figure 1 Typical objects used in 3D geological modelling (A) points, (B) polylines, (C) surfaces and (D) 3D grids. The modelling process usually proceeds from A>B>C>D.

Surfaces are generally interpolated from point and polyline data and this is often the most challenging and critical step in the geological modelling process. For many years, geomodellers have borrowed techniques from the fields of engineering computer aided design (CAD) and 2D Geographical Information Systems (GIS) in which points and polylines are converted into surfaces using simple direct triangulation or explicit geostatistical functions such as kriging (Ringrose and Bentley, 2015). However, while these methods are widely and successfully applied in CAD and GIS they are often less than ideal for 3D geological modelling tasks for a number of reasons:

- 1. Controlling points for a geological surface are often (very) sparse and irregularly distributed.
- 2. Geological models typically consist of multiple vertically-stacked sets of surfaces (stratigraphic horizons) that must maintain a smooth and consistent separation distance (true stratigraphic thickness) while avoiding surface cross-over.
- 3. Controlling points for vertically-stacked surfaces are often inconsistently co-located in the XY plane. This might result from variable borehole depth where a set of horizons are not uniformly proven in all boreholes (Figure 2A). Horizon-by-horizon interpolation of such irregularly distributed datasets has a tendency to create horizon cross-overs (Figure 2B).
- 4. Geological horizons are often cut by structural and stratigraphic discontinuities such as faults and unconformities. Faults impact on multiple horizons generally with a uniform (or smoothly varying) magnitude and direction of offset at each level. Such surface interactions are exceptionally difficult to model using conventional horizon-by-horizon interpolation methods.
- 5. Surfaces representing stratigraphic horizons, faults, unconformities and a bounding volume of interest must intersect precisely to form watertight volumes that can be used to initialise

stratigraphic and structural compartments (regions) within a 3D grid. Such surface interactions are, again, exceptionally difficult to model using conventional horizon-by-horizon interpolation methods

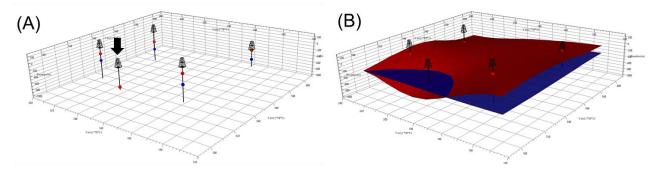


Figure 2 (A) Five wells showing horizon markers for two horizons (red and blue). One well (arrowed) has not reached the blue horizon. (B) Using an explicit surface building method (in this case Discrete Smooth Interpolation) the absence of a blue marker in the arrowed well will create surface cross-over (blue above red) that will require the insertion of corrective phantom points.

While it is possible to overcome most of the problems listed above using explicit surface building approaches, it generally comes at the cost of being hugely time intensive and requiring the manual addition of a large number of 'phantom' points. The addition of phantom points is undesirable not only because of the time requirements but because it can blurs boundaries between hard data points (e.g. well picks) and operator-inserted interpretations, and renders models difficult modify as new hard data becomes available or conceptual ideas change. Primarily for these reasons, in recent years many geomodellers have sought alternative approaches.

## 2.2 A NEW APPROACH: IMPLICIT GEOLOGICAL MODELLING

The use of implicit methods in the creation of 3D computer-generated imagery (CGI) has been around for many decades but until recently its application has been largely confined to computer animation in the film industry. This sector realised at a very early stage in the evolution of CGI that conventional CAD methods used in engineering were unsuitable for the generation of curved, irregular and rapidly changing geometric objects that characterise film animation (Bloomenthal and Wyvill, 1990). Over the past decade a similar train of thought has emerged in the geosciences, driven by the realisation that most geological objects are similarly curved, irregular and problematic to model using conventional explicit methods (Calcagno et al., 2008).

In the Geosciences, implicit modelling has gained traction over recent years and is implemented in commercial software such as Leapfrog, Geomodeller, SKUA-GOCAD, and Petrel (Volumetricbased-modelling). The key feature of implicit modelling that accounts for the growing interest lies in the method by which geological surfaces are constructed. In implicit modelling surfaces are not constructed on an individual horizon-by-horizon. Rather than considering input data on a horizonby-horizon basis implicit modelling uses all of the data simultaneously to interpolate a continuous 3D scalar field that is a representation of the total stratigraphy and structure of a defined volume. Surfaces are then extracted from this implicit field in a subsequent step. Implicit modelling thus counters many of the difficulties described above created by sparse and irregularly distributed input data, that really requires pooling to understand the 3D relationships of a set of surfaces. The implicit method in fact mimics the methods and thought process of a geologist trying to understand the 3D geology of a particular region who will consider all of the evidence simultaneously.

The dataset shown in Figure 2 can be re-visited to expand on how the implicit methods works. In an initial stage, a sealed volume of interest is created that contains a 3D tetrahedral mesh of user defined resolution. All of the input data, which in this case consist of nine well markers from two horizons (see Figure 2A), is loaded into the tetrahedral mesh, generating additional mesh nodes

where necessary (Figure 3A). All of the input data from the two horizons are then simultaneously

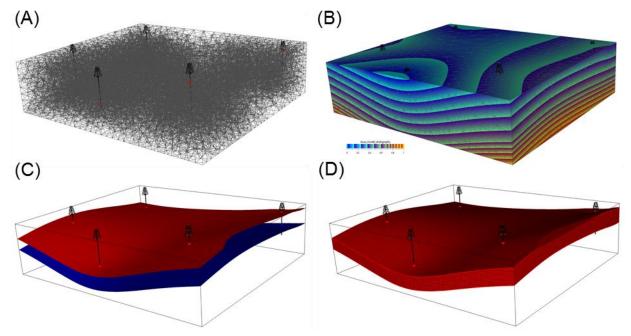


Figure 3 The implicit modelling process, (A) Input data are encapsulated within a Volume of Interest containing a 3D tetrahedral mesh, (D) Input data are interpolated across the mesh producing a 3D scalar field that describes the geometry of the geology, (C) Surfaces are extracted from the scalar field, note absence of horizon cross-over, (D) Surface are used to initialise an irregular 3D gridded volume that can be further discretised using stochastic modelling methods.

interpolated across the mesh to produce an implicit field that represents the structure and stratigraphy of the volume (Figure 3B). This process is guided by a stratigraphic column that defines the relationship between the horizons: the vertical order of stacking and the extent to which horizons are conformable (parallel). The interpolation method varies according to different software. Paradigm SKUA-GOCAD uses discrete implicit modelling to interpolate a piecewise scalar field across the linear tetrahedral elements, while Leapfrog Geo and several other packages use radial bias functions (Laurent, 2016). A description of the mathematical underpinning of the interpolation process can be found in Laurent (2016) and Wellmann and Caumon (2018). Both methods essentially attempt to honour input data while creating a smooth field that minimizes variations in gradient throughout the volume. Stratigraphic horizons are extracted from the implicit field as equipotential surfaces (Figure 3C). Note than any number of infinitesimally closely spaced surfaces could be extracted from the implicit field with the guarantee that horizons will never cross. In the example shown in Figure 3, the implicit function has maintained a plausible stratigraphic thickness between the blue and red horizons without the need to resort to the manual insertion of phantom points in an area where well markers are missing. Surfaces define watertight regions within the volume of interest that can be used to initialize 3D stratigraphic grids (Figure 3D). These can be further discretised using stochastic methods (Ringrose and Bentley, 2015). Greater complexity can be built into the implicit model by inserting faults into the tetrahedral mesh, which act as interpolation barriers, and by defining stratigraphic discontinuities (unconformities) which are used to partition the input dataset and create multiple interpolated functions for each conformable set of horizons.

# 3 Building an implicit geological model of Great Britain

### 3.1 SOFTWARE AND HARDWARE

The modelling was undertaken using Paradigm SKUA-GOCAD (2018) running on a personal computer with Microsoft Windows 10 operating system, Intel Core i7-6700 CPU and NVIDIA Quadro M4000 graphics card. Most of the modelling was carried out using the SKUA Structure & Stratigraphy work-flow.

### 3.2 MODEL BOUNDARIES

The volume of interest was defined as an irregular polygon that broadly encompasses onshore Great Britain with some adjacent offshore regions, most notably the East Irish Sea (Figure 4). The lower boundary plane was set at 15000 m below Ordnance Datum (mBOD) while the upper boundary was set at 1500 m above Ordnance Datum (mAOD). The considerable depth of the model reflects the large elevation range of Proterozoic 'basement' rocks within Great Britain. The model covered an area of 308974 km<sup>2</sup> with a total volume of 5200543 km<sup>3</sup>. All input data and modelling results were held in projected coordinate system OSGB 1936/British National Grid (EPSG:27700). The Z axis of the model was set as positive upwards.

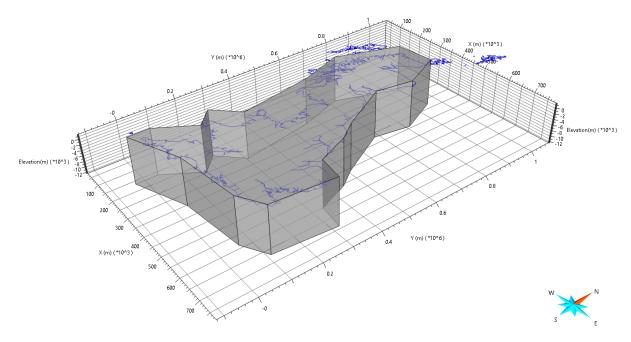


Figure 4 Map showing the bounding polygon (black line) of the modelled volume.

### 3.3 MODEL STRATIGRAPHY

### **3.3.1** The importance of unconformity bound sequences and formation tops

Most stratigraphic sequences can be divided into episodes of broadly continuous sedimentation under steady basin subsidence separated by major breaks which are often, but not always, characterised by tectonic deformation, uplift and erosion (Figure 5). The recognition of unconformity-bound megasequences not only forms a central tenet of stratigraphy (Sloss, 1963) but lies at the core of the implicit modelling process and will fundamentally control the computation of the geological model. This aspect of the modelling in the context of GB is discussed in detail in a following section. Related to the recognition of unconformity bound sequences is the use of formation tops (as opposed to formation bases) in subsurface geological modelling. This standard convention derives partly derives from the fact that wells penetrating a stratigraphic sequence (where it has not been structurally overturned) will enter the top of a formation first and may not exit the lower bounding horizon. However, there is also a strong geological rationale for using formation tops in the context of unconformities and base-lapping sequences. Using formation bases where there is erosion and baselap in a stratigraphic sequence will invariably result in the lower contact of a formation becoming an amalgam of a conformable stratigraphic contact and an unconformity. Two fundamentally different horizons of different origin and age are thus combined. Formations C and D, which form a base-lapping sequence in Figure 5, provide an example. Thus Formation D has a base that includes the conformable contact between D-C and the unconformable contact between D-B. If formation tops are employed Formation D will always have a single conformable contact with Formation E and the horizon top will capture the full extent of the underlying formation.

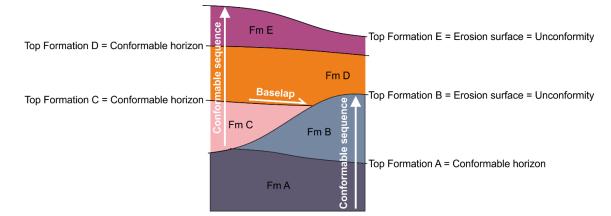


Figure 5 The modelling of unconformities (and their correlative conformities) that bound packages consisting of conformable geological units lies at the core of implicit geological modelling. Unconformities may pass laterally into correlative conformities where sedimentation was essentially continuous.

### **3.3.2** Geological modelling as a two-stage process

A key advantage of the implicit volumetric modelling approach is the output of 3D grids that incorporate all the stratigraphic and structural complexity of the model. Such grids are variably referred to as irregular grids, stratigraphical grids or geological grids and differ from regular (or Cartesian) grids in that, (1) layers of cells conform to stratigraphic horizons, mimicking 'bedding' within the model, (2) cells thicken and thin in response to changes in stratigraphic thickness, and (3) cells are split by faults (Figure 6A). These grids allow the modelling of fine-scale geological properties such as lithofacies using a range of geostatistical and simulation techniques (Ringrose and Bentley, 2015) and open new possibilities for national scale geological modelling as a twopart process. Thus not all stratigraphic units need therefore be modelled at the implicit modelling stage: in any project there will be a critical threshold where switching to grid-based methods becomes more efficient, particularly for units that show strong heterogeneity and lateral facies variation (Figure 6). The aim of implicit modelling is thus primarily to create a structurally-realistic grid that is subdivided into coarse stratigraphic regions (groups and formations). Member and bed scale features can be created using grid-based geostatistics. This has important implications for how we subdivide the stratigraphy of GB and how much we try to incorporate at the implicit modelling stage.

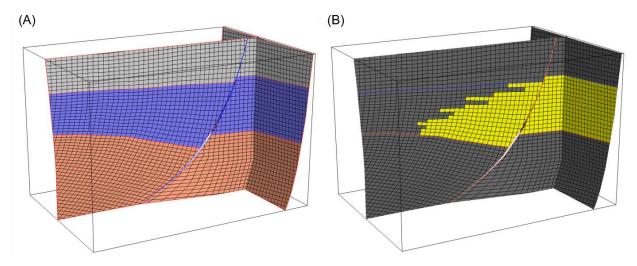


Figure 6 (A) Cross-sections through a 3D geological grid discretised into three formations. (B) Grids allow the modelling of fine-scale properties such as lithofacies that may have complex lateral transitions. Using grid-based methods the purple formation has been further subdivided into two lithosomes (sand and clay).

### 3.3.3 Stratigraphic sequences of Great Britain

Britain has a long and complex geological history dating back some 3 billion years to the Lewisian Gneiss Complex of north-west Scotland and was assembled in a series of terrane collision and accretion events (Brenchley and Rawson, 2006; Trewin, 2002). The literature on UK structure and stratigraphy is vast and only a fraction of this information can be incorporated into large-scale geological models. Moreover the information that is incorporated will depend entirely on the purpose of the model. The work described here has had an emphasis on post-Carboniferous formations in the UK that have greatest impact on groundwater resources (Allen et al., 1997).

As introduced above, the recognition of unconformity-bound stratigraphic sequences is fundamental to the process of implicit geological modelling. In the UK, such sequences are most strikingly seen within compilations of stratigraphic data plotted within a time-space framework (Waters et al. 2007, 2008). Such charts show the fragmentary nature of the stratigraphic record, but also the presence of long episodes of largely continuous sediment accretion separated by lengthy breaks during which time the rock record of the UK was either being destroyed by erosion or was not being deposited (Figure 7). Both the deposition and erosion/non-depositional episodes can be broadly correlated across the UK and show the presence of at least five major unconformities in the Phanerozoic geological record. The unconformities bound a series of (broadly) conformable stratigraphic megasequences. Each unconformity forms a horizon within the implicit model and the underlying megasequences are further subdivided into a number of horizons defined by formation tops (Figure 7). These are described below in order of geological time.

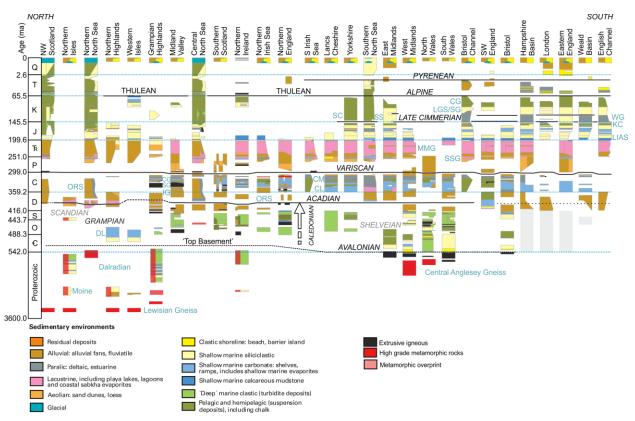


Figure 7 Time-space stratigraphic chart for the UK modified from BGS stratigraphic charts (Waters et al., 2007; Waters et al., 2008).

### 3.3.4 Top Metamorphic Basement

A somewhat arbitrary 'Top Metamorphic Basement' horizon can be created at around the Neoproterozoic-Cambrian boundary that (with some exceptions) brackets the upward limit of strongly metamorphosed rocks in the UK (Figure 7). In southern Britain, on Gondwanan terranes, it overlies Central Anglesey Gneiss and younger (predominantly but not exclusively Neoproterozoic) volcanic and volcaniclastic deposits known from outcrop as the Arton, Longmyndian, Malverns and Charnian complexes (Pharaoh et al., 2011). In Scotland, on Laurentian terranes, the horizon bounds high-grade metamorphic rocks of the Lewisian Gneiss and younger rocks of the Moine and Dalradian supergroups that show strong metamorphic and tectonic overprint from the multiple deformation phases of the Caledonian Orogeny (Figure 7). No attempt has been made to further subdivide this interval of basement rocks.

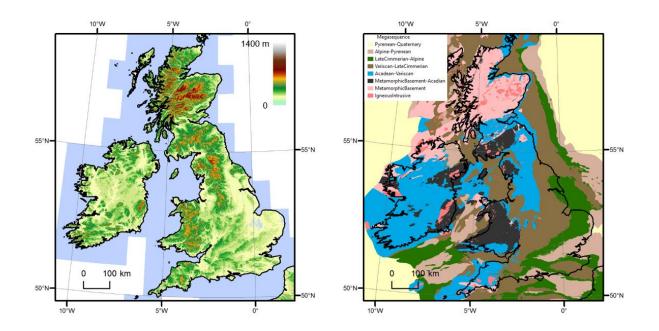


Figure 8 British Isles showing generalised topography and geology, with polygons (modified from Pharaoh et al. (1996)) showing the outcrop distribution of tectonic megasequences onshore and offshore.

### 3.3.5 Acadian unconformity

The Acadian unconformity at around 400 Ma (latest Early Devonian) resulted from the hard collision of Laurentia, Avalonia and Baltica at the end of the Caledonian Orogeny (Mckerrow et al., 2000). Across much of England, Wales and southern Scotland strata between the Acadian unconformity and Proterozoic basement is dominated by fine-grained marine hemipelagic sediments with associated turbidite sandstones and volcanic rocks accumulated in a range of passive margin and back-arc basin settings. Most Silurian marine sequences in the British Isles continue conformably into Early Devonian Old Red Sandstone (ORS) magnafacies (Mckerrow et al., 2000): the Acadian Unconformity occurring within this fluvial-dominated red-bed succession. The Acadian unconformity is a major hiatus with extensive uplift, erosion and redistribution of pre-Acadian deposits (Soper and Woodcock, 2003). In areas such as Lancashire, Yorkshire and Cheshire Carboniferous Limestone rests unconformably on Silurian strata. No attempt has been made to model subunits within this sub-Acadian Early Palaeozoic interval.

### 3.3.6 Variscan unconformity

The Variscan unconformity resulted from the oblique collision of Gondwana and Laurussia on Britain's southern flanks (Kroner and Romer, 2013). Compression and uplift of the Variscan foreland produced widespread erosion and non-deposition across Britain and Ireland recorded in the extensive unconformity below Permian sequences. The Acadian-Variscan megasequence contains a heterolithic assemblage of facies that accumulated in a number of depocentres located between highs that included the Scottish Highlands, Southern Uplands, Alston Block and Welsh-Brabant Massif (Brenchley and Rawson, 2006).

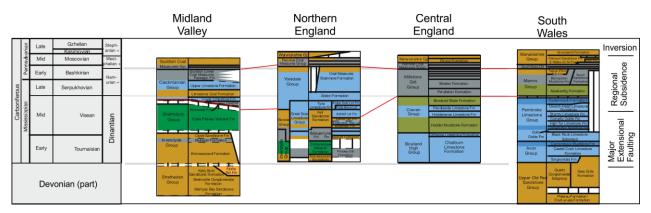


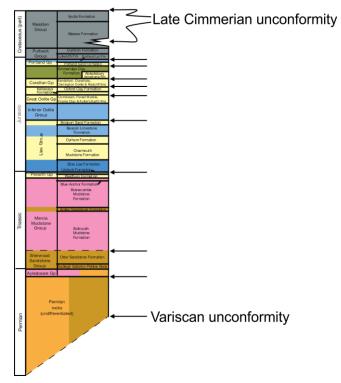
Figure 9 Carboniferous stratigraphy (Waters et al., 2007; Waters et al., 2008) in four areas of Great Britain showing position of modelled horizons (red) within the Acadian-Variscan megasequence. No chrono- or lithostratigraphic correlation is implied by the red lines linking columns.

In very general terms, the stratigraphy of the megasequence records an upward stratigraphic trend from Devonian terrestrial deposits, into early Carboniferous (Dinantian) shallow marine carbonates (and correlative deep marine mudstones), to late Carboniferous fluvio-deltaic deposits (Namurian) and coal measures (Westphalian). In areas north of the Alston Block (e.g. Northumberland-Solway Basin and Midland Valley of Scotland) marine carbonates appear later in the Yoredale and Clackmannon groups with the Dinantian dominated by fluvial, lacustrine and volcanic accumulation of the Inverclyde, Strathclyde and Border groups. The development of extensional basins and blocks dominated the depositional framework of the Acadian-Variscan megasequence, particularly during the Dinantian. Namurian and Wesphalian fluvio-deltaic deposits are generally considered post-rift, with an increasing importance of compressional basin inversion associated with Variscan mountain building toward the end of the Carboniferous. Horizons mapped on seismic reflection and borehole data within the Acadian-Variscan megasequence have typically included locally significant limestone formations within the Dinantian (e.g. Chatburn Limestone) and major (diachronous) facies changes at around Top Dinantian (base Millstone Grit) and Top Namurian (base Coal Measures) (Kirby et al., 2000; Pharaoh et al., 2011; Smith et al., 2005). In the Northumberland-Solway Basin additional horizons are typically mapped at the top (and within) the mixed volcanic and terrestrial-dominated deposits of the Dinantian Inverclyde and Border groups (Chadwick et al., 1995). In the Midland Valley of Scotland horizons are typically mapped at a number of group (Strathclyde, Clackmannan and Coal Measures) and formation boundaries (Underhill et al., 2008). Two subdivisions are used in this work at (or around) Top Dinantian and Top Namurian. Due to much lateral facies variation, further subdivision of this megasequence can probably be more effectively achieved by on grid-based methods.

### 3.3.7 Late Cimmerian unconformity

The Late Jurassic and Early Cretaceous was characterised by series of uplift and erosion events that developed a complex set of unconformities, generally referred to as the Late-Cimmerian unconformity. The unconformities are not related to an orogenic event but localised regional uplifts. Along the east coast of England, on the flanks of the southern North Sea Basin, Jurassic strata are truncated within the Kimmeridge Clay and unconformably onlapped by Early Cretaceous formations such as the Speeton Clay, Spilsby Sandstone and Carstone (Cameron et al., 1992). In the Wessex Basin of southern England, uplift of the Cornubian ridge in the Berriasian, related to the onset of sea-floor spreading in the Bay of Biscay, imparted a strong easterly tilt and progressive westward truncation of pre-Aptian formations down to the Palaeozoic (McMahon and Turner, 1998). The rapidly subsiding Weald Basin formed a sink for much of the eroded material. Elsewhere in Britain, Jurassic and Cretaceous strata (and any evidence they contain for the Late Cimmerian unconformity) have been largely obliterated by later erosion (Figure 7).

The Variscan-Late Cimmerian megasequence was largely deposited in a series of extensional rift basins, many of which were controlled by reactivated Caledonian and Variscan fault structures. An initial terrestrial fill of Permian to Triassic siliciclastic and evaporitic red-beds passes upwards into a Jurassic sequence of alternating marine mudstones, sandstones and carbonates with a switch to siliciclastic-dominated paralic environments in the Early Cretaceous. The succession is generally conformable, base-laps the Variscan unconformity and, for the purposes of modelling, has been divided into nine horizons at major formation or group-level boundaries (Figure 10).



# Figure 10 Modelled horizons shown by black arrows in the Late Cimmerian-Variscan megasequence

### 3.3.8 Alpine-Thulean unconformity

The Alpine-Thulian unconformity occurs around the Cretaceous Tertiary boundary and records the complex (and much debated) interactions between northward-directed crustal compression related to Alpine orogenesis, ridge push from North Atlantic spreading, and epeirogenic uplift resulting from igneous underplating and the Iceland mantle plume (Cogné et al., 2016). Regional epeirogenic uplift was centred in northern Britain coincident with British Tertiary Igneous Province (Łuszczak et al., 2018), while the strongest effects of short wavelength folding and faulting around the Cretaceous-Tertiary boundary are seen in the southern North Sea Basin (Hibsch et al., 1993). Erosion of the Chalk Group of southern England may have been largely (or partly) a consequence of marked eustatic sea-level fall at around the Cretaceous-Tertiary boundary (Hallam and Wignall, 1999). The main compressional inversion of the Wessex Basin in southern Britain did not occur until the late Oligocene and Miocene (Newell and Evans, 2011) and was probably driven by Pyrenean compression (Parrish et al., 2018). Across northern Britain regional denudation associated with mantle-plume activity resulted in the erosion of up to 2.4 km of rocks (Łuszczak et al., 2018; Tiley et al., 2004), shaping the geomorphology and outcrop distribution that is seen today, with late Mesozoic and Cenozoic deposits preserved mainly in southeast Britain.

The Late-Cimmerian-Alpine/Thulean megasequence records the stratigraphic signal of Cretaceous eustatic sea-level rise and a switch from syn-rift to post-rift tectonic control. Two horizons were picked for the purposes of modelling: Top Weald Group and Top Selborne Group and their broad lateral equivalents (Figure 11). The Top Weald sequence included marked lateral changes in facies from paralic south of the London Platform to shallow marine on the north of this divide, with finer-grained deeper water facies in the Cleveland Basin. The Top Selborne Group is coincident with

the Cenomanian transgression and overlies an interval of marine deposits with marked lateral facies change. The Top Alpine-Thulean horizon forms the top of the Chalk Group deposited during maximum eustatic sea-levels that flooded the London Platform.

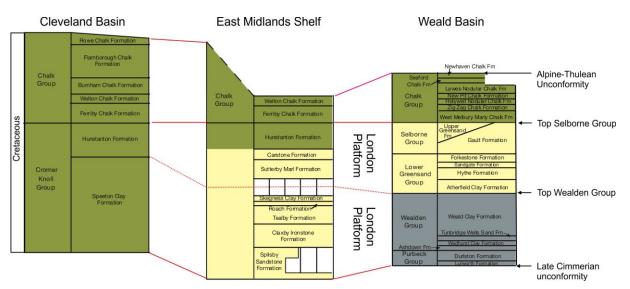


Figure 11 Modelled horizons within the Late Cimmerian-Alpine/Thulean megasequence. No chrono- or lithostratigraphic correlation is implied by the red lines linking columns.

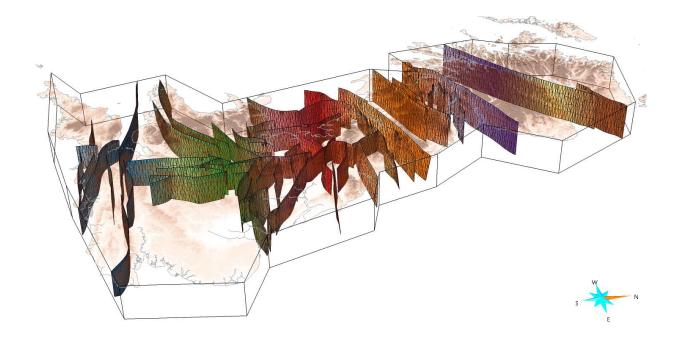
### 3.3.9 Pyrenean unconformity

The Pyrenean unconformity represents a major northward-directed compressional event that occurred in the late Oligocene and Miocene coincident with Pyrenean mountain building (Parrish et al., 2018). It produced folding, normal fault inversion and localised kilometre-scale uplift and erosion in southern Britain. The unconformity caps the 'Tertiary' deposits of Britain that are largely (but not exclusively) preserved within the synclinal cores of the Hampshire and London basins. Tertiary deposits are conventionally considered the youngest bedrock deposits of Britain. They are unconformably overlain by a patchy distribution of Quaternary superficial deposits that are discussed in more detail below. Tertiary deposits have not been further subdivided within the implicit model but there is considerable scope for grid-based refinement of this interval.

### 3.4 MODEL INPUT DATA

### 3.4.1 Fault network

The model uses a simple fault network based primarily on the Tectonic Map of Britain, Ireland and adjacent areas (Pharaoh et al., 1996). The faults only include those that represent major basinbounding structures and are modelled as simple vertical or inclined planes (Figure 12). Fault planes form discontinuities in the 3D implicit field, controlling the introduction of cuts and structural offset in stratigraphic horizons.



### Figure 12 Illustration of the simplified fault network used in the model.

Faults modelled as simple planes are of course often gross simplifications of geological reality where faults consist of multiple segments that branch, splay and interact in a broad fault zone (Figure 13). Many Cenozoic and Mesozoic faults in the UK formed above deep basement structures of Caledonian and Variscan age that were repeatedly reactivated as normal, reverse or strike-slip faults depending on the ambient stress field (Peacock, 2009). In areas such as the Weald Basin, Variscan thrusts often show complex reactivation styles with multiple hanging-wall cut-offs developed during extension and low-angle footwall cut-offs during later compression (Figure 13).

In Great Britain many faults in the Wessex and Weald basins are observed to terminate at the late Cimmerian unconformity (Mathers et al., 2014) and for simplicity this rule has been applied to all faults in the model. Note however there is good evidence for fault offset in post late Cimmerian strata (Chalk and Tertiary) in areas such as the London Basin (Mathers et al., 2014).

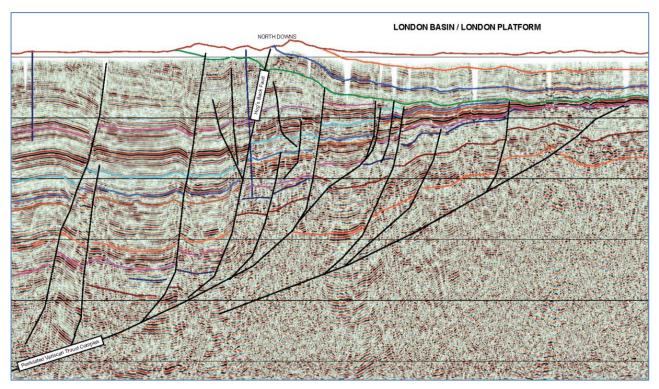


Figure 13 Interpreted seismic reflection profile across the southern margin of the London Platform showing a Variscan thrust that was extensionally reactivated as a normal fault zone in the Mesozoic and compressionally reactivated in the Cenozoic. Field of view is approximately 15 km wide and 10 km deep and is modified from Butler and Jamieson (2013). Note fault termination at the Late Cimmerian unconformity (green pick).

### 3.5 DIGITAL TERRAIN MODEL

OS Terrain 50 is the topographic surface used in the model. OS Terrain 50 is available through OS OpenData<sup>TM</sup> and can be downloaded as an ASCII grid with a 50 m horizontal grid resolution. In the model topography represents the uppermost unconformity, against which many dipping geological horizons are truncated. Such truncations represent the crop-lines shown on geological maps. In offshore areas the 2018 version of the European EMODnet bathymetric model at a grid resolution of 1/16 \* 1/16 arc minutes (circa 115\*115 m) has been used to model seafloor topography (http://www.emodnet-bathymetry.eu).

The spatial resolution and surface roughness of terrain data is generally much higher relative to the other types of geological data used in the model. Terrain data may have a spacing on the order of metres or less, while boreholes may be spaced at kilometres or more. For large models this can create problems because the density of the tetrahedral mesh across which the implicit function is interpolated cannot currently be varied throughout a model. For large models, a single value must be chosen that is a compromise between a reasonable model build time and preserving sufficient resolution on the terrain and other model surfaces. Experimentation shows that the horizontal resolution of the tetrahedral mesh should in general not exceed 10 times the data spacing to maintain an acceptable terrain model (Figure 14). A horizontal resolution of around 500 m was thus used in many of the model runs which results in some smoothing of the terrain data.

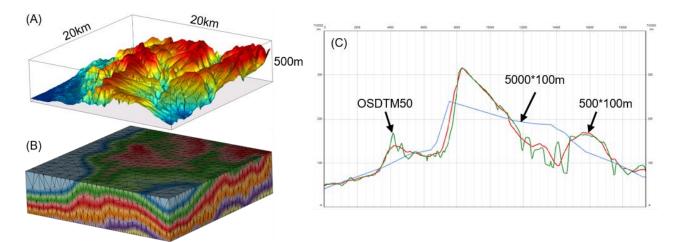
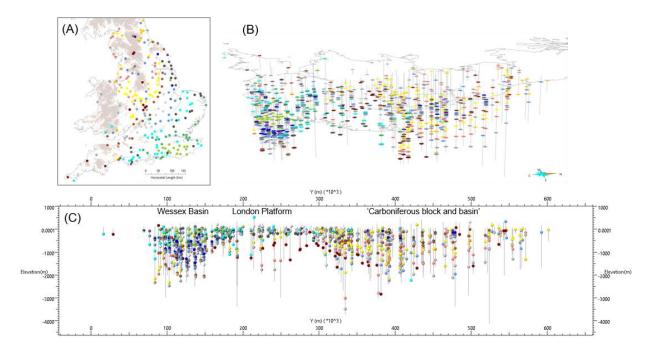


Figure 14 (A) Sample of OS Terrain 50 (North York Moors) on 50 m data posting. (B) 3D scalar field interpolated across a tetrahedral mesh using terrain model as input. (C) Cross-section comparing results of the extracted modelled horizon with OS Terrain 50 at different horizontal mesh resolutions, vertical resolution is kept constant at 100 m. A mesh resolution of 50 m produces a near identical result (not shown), while horizontal meshes at 10 and 100 times the 50 m data spacing produce lower resolution terrain models.

### **3.6 BOREHOLES**

The model currently uses the same borehole dataset as UK3d\_v2015 (Waters et al., 2015) which are largely a subsample of the <u>BGS Stratigraphic Surfaces Database</u>. Presently the boreholes cover England and Wales only and represent only a fraction of the data gathered from deep hydrocarbon, coal, geothermal and hydrogeological activities over many decades. Borehole spacing is generally in the order of 10-30 km and most boreholes terminate at elevations above -2000. The broad geological structure of England and Wales is clearly illustrated by a plot of borehole total depth mBOD (Figure 15). Borehole paths are currently set as vertical, which is a reasonable approximation for the vast bulk of the dataset. However, these should be replaced with deviated paths where well deviation has a significant impact on marker elevation and the information is available. Well markers are located where the well path crosses a geological horizon. For the purposes of modelling, well markers are assigned to formation tops and wells are classified using the working stratigraphic column. The well stratigraphy is an integral part of the modelling process allowing, for example, the identification of locations where horizons have not been intersected by a well path and must therefore lie below the terminal depth.



# Figure 15 (A) Map showing distribution of boreholes, (B) Perspective view of borehole markers, (C) Borehole data viewed vertically from the east showing variations in total depth.

Most of the downhole stratigraphic picks were taken as recorded in BGS datasets. However, ideally these should be verified and adjusted using geophysical log data and well correlation panels (Figure 16). This has been partially carried out for some units such as the Chalk Group, Oxford Clay and Sherwood Sandstone but needs to be extended to all parts of the stratigraphic column (Newell, 2018; Newell et al., 2018).

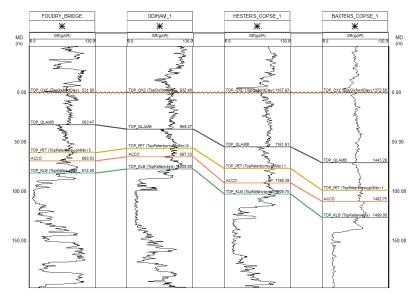


Figure 16 Example of a well panel showing high-resolution correlation of the Oxford Clay using gamma-ray curves. Section is flattened on the top of the Oxford Clay.

### 3.7 EXISTING CROSS-SECTIONS

Pre-existing cross-sections from a range of BGS maps (Pharaoh et al., 1996) and memoirs (Kirby et al., 2000) have been georeferenced in 3D (Figure 17) and provide a valuable source of subsurface information. In particular many of the sections from the Tectonic Map (Pharaoh et al., 1996) incorporate the results of the British Institutions Reflection Profiling Syndicate (BIRPS) who shot approximately 12,000 km of deep, multi-channel seismic reflection data around the British Isles from 1981 to 1991 during 14 surveys (Brewer et al., 1983). Recording depths vary depending on the purpose of the survey but range from 15-40 seconds two-way time. These lines

provide an important source of information on the deep crustal structure of the British Isles and surrounding continental shelf. 3D polylines have been captured directly from the cross-sections and used as input data in the modelling.

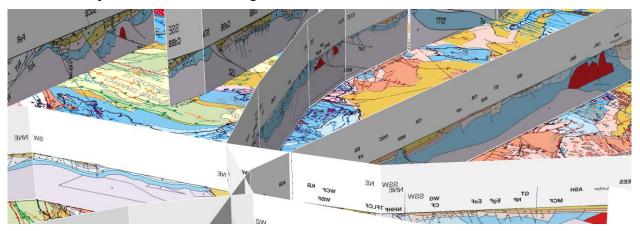
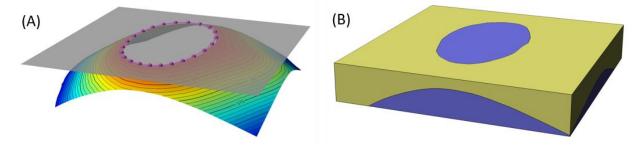


Figure 17 Pre-existing cross-sections georeferenced and displayed in a 3D window

### 3.8 OUTCROP AND SUBCROP DISTRIBUTION MAPS

Mapped lines on geological map show the intersection of a geological horizon with the topography and define regions on the topographic unconformity where a geological unit is present or has been eroded (Figure 18). Using geological map polygons to define areas of erosion can be useful and rapid means of ensuring the model honours the mapped distribution of a geological unit. For national scale geological modelling the BGS 1:625 000 scale Bedrock North and South maps (DiGMapGB-625) are generally adequate. As discussed above, surface topography is just one of a sequence of major unconformities that control the distribution of geological units across Britain. BGS has prepared maps showing the distribution of units below and above the Late Cimmerian, Variscan and Acadian unconformities and these form an important source of information for subsurface modelling. The erosion history of most geological units is controlled by multiple unconformities creating complex geometries.



# Figure 18 (A) The erosion outline (pink polygon) is used to constrain the area where the top of the blue geological unit (B) has been eroded at the unconformity.

Geological map (outcrop) polylines can also be combined with subcrop information to create outlines showing the non-erosional or depositional limits of a geological unit. Depositional outlines might for example constrain the extent of a base-lapping horizon on an irregular unconformity (Figure 19). The generation of these total coverage polygons is generally a highly iterative process that is closely tied to the modelling process. It is often better to initially (or entirely) omit constraints such as depositional outlines and allow the formation limits to be derived computationally. This can provide insight into possible patterns of formation coverage that were not initially considered by the geomodeller.

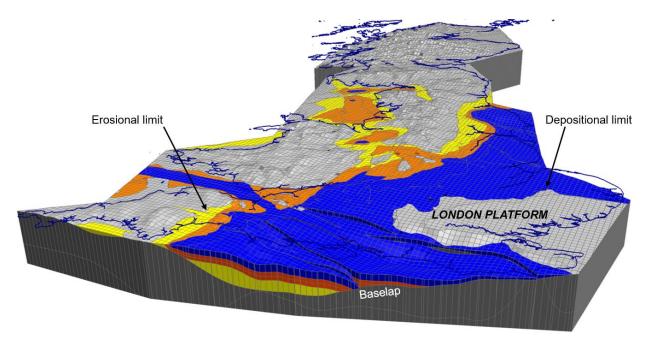


Figure 19 Baselap patterns of Triassic and Lower Jurassic strata on the sub-Variscan unconformity around structures such as the London Platform can be generated computationally or by the use of depositional outline polylines

### 3.9 SEISMIC REFLECTION DATA

Seismic reflection data are available in a number of forms suitable for modelling. Depth-converted structure maps are available for most sedimentary basins in the UK, although data coverage is often patchy. Some of the best coverage exists across the Carboniferous basin and block provinces of central England (Kirby et al., 2000; Pharaoh et al., 2011; Smith et al., 2005) and northern England (Chadwick et al., 1995). Much of the depth-converted data for these, and other studies, is stored in the Seismic Locations and Sections database (LOCSEC) which holds digitised seismic reflection survey location and line-interpretation data. The data are grouped by interpretation project area. Interpreted regional seismic reflection profiles from sources such as the UK Onshore Geophysical Library (Butler and Jamieson, 2013) provide a useful guide to regional structural trends and stratal relations even if the depth conversion should be regarded as approximate. 3D seismic can provide high-resolution structure maps, although coverage at the UK scale is sparse. Horizon elevation interpretations from seismic reflection data can show considerable departure from data such as boreholes because of the relatively coarse resolution of seismic data and uncertainties associated with time to depth conversion. This can be accommodated within the implicit modelling routine by using seismic data as a 'soft constraint' that guides the structural form of a surface but does not control its elevation.

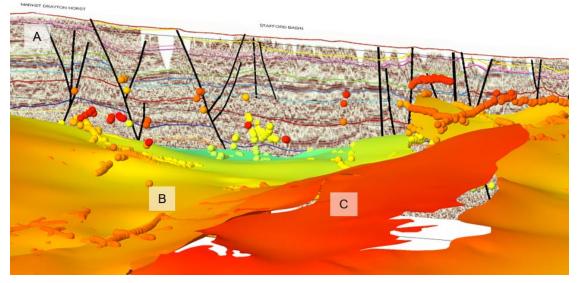


Figure 20 Seismic data in three forms (A) interpreted seismic profile, (B) Depth converted seismic picks as points, (c) Surface interpolated from depth converted seismic.

### 3.10 DIGITISED CROSS-SECTIONS

Manually constructed cross-sections are an important model input, providing horizon and fault input data where none exists and playing a key role in distilling a range of inherently fuzzy input datasets into a single interpretation that incorporates the geological expertise (or erroneous opinions) of the geomodellers (Figure 21). For example, surfaces based on seismic, outcrop intersections, structure contour sets and pre-existing models can be displayed in a 2D cross-section window and refined into a new interpretation. Section construction and modelling is a highly iterative process whereby the results of the implicit model are displayed in the 2D section window and used to inform where interpreted input data needs to be added, removed or modified. The polyline picks are regarded as soft data and the degree of fit (smoothing) of modelled horizons to the data can be adjusted. Ideally, the density of manually digitised data should be kept to the absolute minimum amount required to generate acceptable surfaces so that models are maintained in a form that is easy to edit.

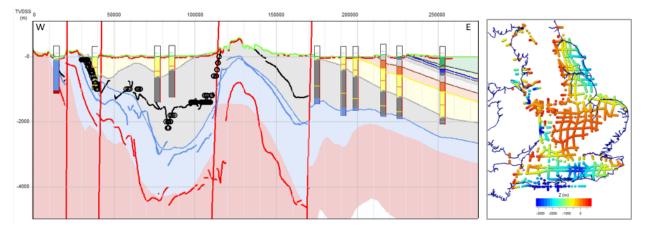


Figure 21 A typically 'noisy' cross-section window combining datasets that include terrain, rockhead, surfaces derived from seismic interpretation, boreholes and pre-existing structure contours. Such datasets can be cleaned and combined into new horizon picks (digitised polylines) that are used as input data for implicit modelling. The model can be displayed as a background image in the window starting a (usually lengthy) iterative process of data editing and modelling. Map shows polylines used in the creation of the Variscan unconformity horizon that were created on a grid of cross-sections.

### 3.11 BEDDING DIP AND AZIMUTH

Structural measurements can be an important means of constraining the shape of the implicit field and, in fact, are one of the key reasons why implicit modelling has gained traction in mining geology and other sectors that commonly encounter highly-deformed rocks (Figure 22). Structural measurements may represent conventional 'dip and strike' information obtained from outcrop and shown on geological maps. Alternatively, they can be acquired from boreholes where highresolution, orientated images of the borehole wall are generated by optical, acoustic or electrical geophysical tools (Poppelreiter et al., 2010). Structural data have not been used extensively during the work described here simply because (in BGS) most structural data of this type has not yet been captured digitally from geological maps and the number of boreholes with image logs (or interpreted image logs) is limited. However these data are potentially important, both in terms of model construction, and in validating modelled surfaces through comparison of modelled and observed dip/azimuth values.

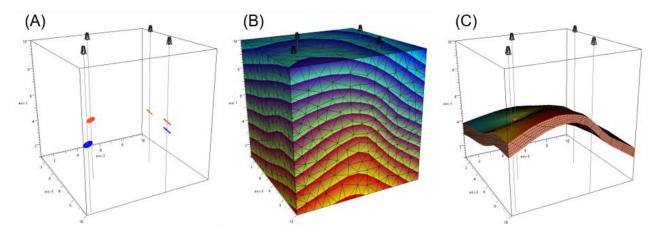


Figure 22 (A) Five well markers that carry dip and azimuth data in four wells across two horizons (red and blue). (B) The structural data carried on the markers are used to shape the 3D scalar field representing the structure-stratigraphy model. (C) Surface and gridded volumes are extracted from the scalar field.

### 3.12 INTRUSIVE IGNEOUS BODIES

Intrusive igneous bodies occupy a relatively large volume of the UK crust (just how much could be determined by a 3D geological model) occurring both exposed at surface and concealed beneath sedimentary overburden (Figure 23A). They have a broad range of ages and compositions, but the bulk are associated with convergent plate tectonic events associated with the Caledonian and Variscan orogens or magmatic activity linked to North Atlantic spreading in the early Tertiary (Brenchley and Rawson, 2006). Igneous intrusions, and comparable geological features such as salt domes, do not follow conventional rules of stratigraphic superposition. An intrusive body is a "geologic event" whose cross-cutting relationship to other layers cannot be explained in terms of normal stratigraphic relationships such as conformity, erosion or baselap.

The modelling of igneous intrusions can be approached in a number of ways. A simple method is to omit intrusive bodies from the implicit modelling stage and then 'burn' the igneous intrusions into the gridded output afterwards. This simply involves replacing rock properties in grid cell regions (most probably on a regular grid) that occur within the intrusive volume. Figure 23B shows a simple example where intrusive bodies have been inserted into a coarse gridded geological model of the UK using information on, (1) their outcrop distribution, (2) their subsurface extent and (3) depth limits. Most of the data have been derived from the BGS Tectonic Map and associated regional scale crustal cross-sections (Pharaoh et al., 1996).

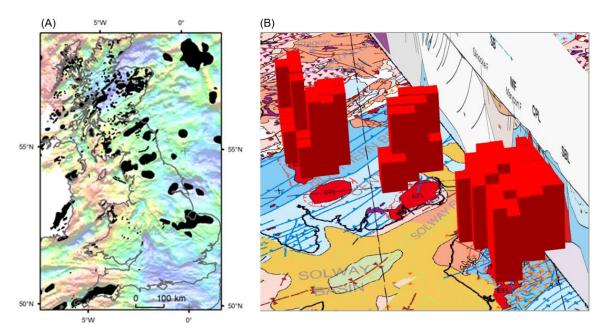


Figure 23 (A) Igneous intrusions at outcrop and subcrop shown as black polygons based on Pharaoh et al. (1996). Background map shows BGS colour shaded-relief image of the <u>UK</u> gravity field. (B) Simple modelling of igneous bodies based on map and cross-section extent shown in Pharaoh et al. (1996).

A second approach is to include intrusive bodies within the implicit model building process, where they effectively create blanked areas within the scalar field across which stratigraphic horizons are terminated and excluded (Figure 24). This requires the creation of closed surfaces that define the shape of the intrusive body: there are clearly many uncertainties in this process some of which might be reduced by detailed analysis of gravity data (Taylor, 2007).

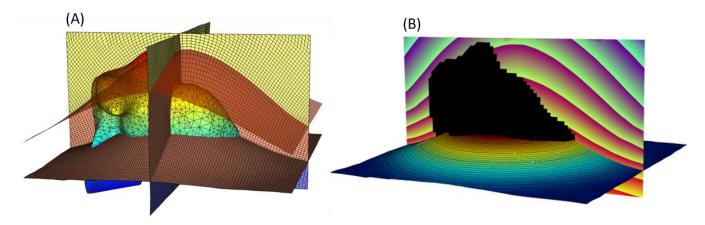


Figure 24 (A) Hypothetical intrusive body constructed from a triangulated mesh surface. Abutting stratigraphic horizons terminate against the intrusive body and do not pass through it. The implicit modeller ensures that all contacts are sealed despite the complex geometry. (B) Cross-section through the 3D stratigraphic function showing blanked area within the volume occupied by the intrusion.

### 3.13 DATA RELATING TO SUPERFICIAL DEPOSITS

The last 2.4 million years has been dominated by alternating glacial and interglacial cycles and deposits associated with the most recent Anglian and later Devensian can be found across the UK (Dearman et al., 2011). The landmass of Great Britain can be divided into two distinct provinces,

based on the glaciation limits, geomorphology, and the nature and distribution of superficial deposits (Figure 25). A 'non-glaciated province' lies south of the known limit of the Anglian glaciation while a 'glaciated province' is located to the north of this line (Booth et al., 2012). The two provinces can be further subdivided into Quaternary domains characterised by particular elevation ranges, erosional geomorphic features and changes in the relative proportion of glacigenic, fluvial, lacustrine, aeolian, marine, organic and periglacial deposits (Booth et al., 2012). Boreholes show that Quaternary deposits range up to about 150 m thick, but over most of Great Britain they are typically 5 m or less in thickness (Lawley and Garcia-Bajo, 2010). Notable areas of thick Quaternary deposits occur within the low-lying basins and coastal margins of central England (Figure 25).

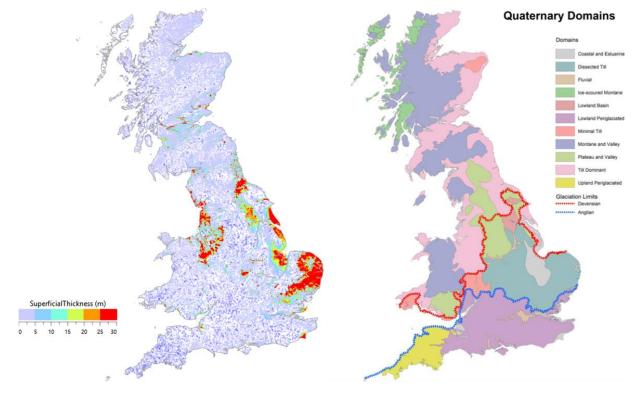


Figure 25 Superficial deposits thickness map (Lawley and Garcia-Bajo, 2010) and superficial domains of Great Britain (Booth et al., 2012).

Quaternary deposits are often (but not always) heterogeneous with a complex sedimentary (and glaciotectonic) architecture that is challenging to model. While deterministic modelling methods have often been successfully employed (Burke et al., 2014), such characteristics tend to encourage the use of grid-based modelling methods that involve geostatistical interpolation or simulation (Janszen et al., 2013; Kearsey et al., 2015). While it is entirely feasible (and is generally desirable) to integrate bedrock and superficial deposits within a single implicit model (Newell et al., 2015a) it is debatable whether this is the most efficient approach on a national scale, simply because of the small cell dimensions (and thus large number of cells) required to capture the relatively thin, heterogeneous superficial cover. One approach toward integrating bedrock and superficial geological models might be to construct independent models and then merge geological properties on a separate regular grid. Figure 26 shows an example of a gridded superficial model created relatively simply by selecting cells that occupy the volume between rockhead and topography and then further discretising the 3D grid using BGS Quaternary domains, effectively combining the two datasets shown in Figure 25. The grid could clearly be refined using other map and borehole datasets. Where bedrock models have been constructed using topography rather than rockhead as the upper bounding surface, cells in the merged grid will have their bedrock properties overwritten by superficial properties.

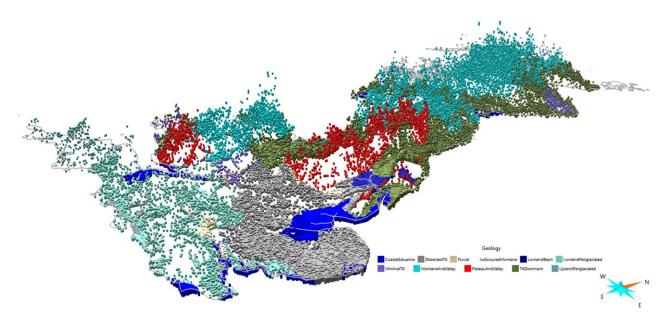


Figure 26 Superficial geology model generated by selecting grid cells in a region defined by rockhead (base of superficial deposits) and topography. The selected cells were further discretised using superficial domain polygons. Regular gridded data of this type can be readily merged with grids carrying a bedrock property.

## 4 Model construction

## 4.1 MODEL WORKFLOW

As implemented in Paradigm SKUA-GOCAD 2018, implicit modelling is a work-flow driven task that systematically works through a number of stages (Paradigm, 2015). The stages are described in full in software documentation, in brief:

- 1. Create a stratigraphic column and define stratal relationships (conformable/unconformable /erosion/baselap).
- 2. Select well and other stratigraphic horizon input data and define the modelling role of each object.
- 3. Select fault input data, define the modelling role of input data, assign the throw of faults where known and establish relationship of faults to unconformities.
- 4. Define any intrusive boundary features.
- 5. Compute a volume of interest (VOI).
- 6. Create a fault network within the volume of interest and establish topological relationships (crossing, branching, intersection).
- 7. Creating a 3D tetrahedral mesh within the VOI of a specified horizontal and vertical resolution.
- 8. Interpolate input data to create 3D scalar fields that represents a structural-stratigraphic model within the VOI. The degree of smoothing (fit) between input data and the interpolated field can be user specified.
- 9. Extract horizons from the scalar field.
- 10. Build the geological grid of a specified cell size.

The modelling process is invariably a highly iterative process whereby insights gained during the 3D visualisation and modelling lead to modifications in the underlying conceptual model and the 'soft' input data.

## 4.2 ERROR CHECKING

The workflow has in-built functionality to check for errors and inconsistencies (e.g. incorrect well stratigraphy, well paths crossing fault planes without an associated fault marker) at all stages of the workflow. Maps and tables are generated to analyse fit error between horizons and input data. Maps can be created to check for anomalous changes in thickness that might indicate modelling errors or incorrect input data. In SKUA-GOCAD uncertainty envelopes can be calculated for both horizons and faults (Evile, 2018) although the value of this information has not been tested in this work. Uncertainty remains an unresolved issue in geomodelling because much of the input data is interpretative and the underlying geological systems are chaotic.

## 4.3 MODELLING METADATA

Most geomodelling software is now capable of capturing metadata on model objects and the modelling process within the application. In SKUA-GOCAD the original source can be appended to objects and all edits on the object from the time of import onwards are systematically logged. All input data and model input parameters used within the implicit modelling workflow are recorded and can be exported as an HTML document. Input data that were used in the modelling are precisely recorded, including parts of the dataset (e.g. inconsistent points) that were discarded during the modelling process. Multiple modelling 'scenarios' can be generated using different subsets of the modelling input data without permanently modifying the integrity of the original dataset in any way. Input data are clearly distinguished from modelled results at all stages of the modelling process.

# 5 Model outputs

## 5.1 CONVENTIONAL OUTPUTS

The modelling creates a range of 'conventional' geological outputs that includes surfaces, structure contour maps, thickness maps, cross-sections and well correlation panels (Figure 27). Most of these outputs are a by-product of the modelling work-flow, for example, well correlation panels provide marker inputs and thickness maps are created to error check horizons. The link between modelling process and product is thus both seamless and highly iterative. All horizon grids generated by the implicit modelling process can be converted to triangulated surfaces or 2D ASCII grids for export to other software.

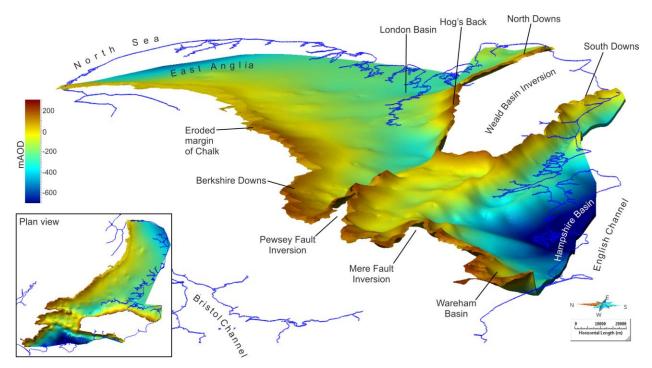


Figure 27 Modelled structure of the Chalk showing W-E trending inversion anticlines south of the London Basin (Newell et al., 2018).

### 5.2 3D STRATIGRAPHIC GRIDS

With conventional explicit surface-based modelling approaches, the creation of 3D stratigraphic grids has always been a separate, time-consuming and often extremely challenging task. Implicit modelling has revolutionised the creation of 3D stratigraphic grids. With the adoption of a volumetric modelling approach irregular grids that conform to the stratigraphic and structural fabric of the geological model are created as an integral part of the work-flow. Edits to well markers, faults, horizons or other input data can thus be readily mirrored in the derivative 3D stratigraphic grid. The stratigraphic grid is 'geostatistics-ready' and has important applications in, (1) the modelling of lithofacies and other rock properties, (2) the integrated visualisation and analysis of rock volumes with other 3D scalar fields such as subsurface temperature, and (3) the transfer of static geological properties into dynamic flow and geomechanical models. Stratigraphic grids are primarily used for the accurate modelling of rock properties related to the stratigraphy. In most cases, irregular stratigraphic grids are transformed into regular grids (by a process of property transfer that may involve upscaling) to provide interoperability with other software.

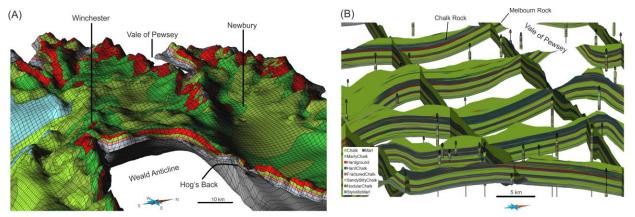


Figure 28 (A) Gridded stratigraphic model of the Chalk Group subdivided into lithostratigraphic regions. (B) Cross-sections through the grid showing lithofacies property interpolated across the grid

## 6 Discussion

### 6.1 ADVANTAGES AND DISADVANTAGES OF IMPLICIT MODELLING

Implicit geological modelling is a developing field but one that has gained considerable traction in recent years (Wellmann and Caumon, 2018). In many ways the key strength of the method is its capacity to replicate the cognitive process of the geologist attempting to understand the structure and stratigraphy of a particular volume of the Earth's crust, thus all geological evidence is considered together (analogous to creating a volumetric implicit function) and known stratigraphic and structural rules are applied. By automating some of the modelling process a number of benefits are realised including, (1) models can be built more rapidly, (2) geometries can be created that are simply too complex for manual digitising, (2) by reducing the number of phantom points models are easier to update and edit, (3) the ratio of time spent building models to time spent considering their geological implications is much improved, and (4) the modelling algorithms may produce a solution, that because of operator bias and experience, had not previously been considered. Cowan (2016) has written an astonishing article on just how extreme and entrenched operator bias can be within the geosciences.

Geological model automation does of course not come without its costs. It can be extremely challenging to convert geological data and conceptual ideas into a corresponding 3D model using automated approaches. Even relatively simple tasks, such as maintaining a smooth, consistent stratigraphic thickness within a stack of conformable surfaces can sometimes produce disappointing results, highlighted by upright or inverted cones where horizons have been force-fitted around well markers (Laurent, 2016). There is also the ever present danger that implicit models, which can be rapidly produced and can superficially appear polished, are entirely erroneous. Reid (2007) outlines examples from the mining sector where implicit models generated without due attention to robust geological principles are leading to overestimates of mineral resources that are damaging to future investor confidence.

### 6.2 DO WE NEED GEOLOGICAL MODELS AT A NATIONAL SCALE?

Most geological modelling tasks tend to address a particular problem at a specific site such as an oilfield, mine, or groundwater contamination zone. Such sites might cover a relatively small area in the range 1-100 km<sup>2</sup>. Implicit modelling methods have been shown to produce good results (on the basis of new drilling on well prognoses) when applied to relatively small rock volumes, primarily because meshes can be used at a high resolution (Newell et al., 2016; Newell et al., 2015b). As a rule, geomodellers should always preferentially work within the smallest possible volume of interest.

National scale models will invariably be a compromise between having a mesh resolution that allows an acceptable fit to input data while maintaining reasonable model computation times. The only rationale for creating a model at a national scale is therefore that this scale of model is actually required. Such reasons might include:

- 1. Geological investigations into large-scale depositional trends within a particular unit or time-slice across several depositional basins (Newell, 2018).
- Property modelling across large areas or geological units where, (1) time efficiencies are gained by reducing the number of model regions and operations that need to be performed, (2) Model boundary effects and misfit across boundaries need to be avoided.
- 3. Large scale investigations between rock units and other properties such as geothermal or groundwater chemistry.
- 4. Where modelling on a national scale improves the geological model by eliminating boundary effects or increasing the size of a low-density input dataset.

In other cases, modelling on the smallest possible volume of interest is the optimum approach. In many respects, the relative ease with which semi-automated implicit models can be built changes

the geomodelling paradigm. Models do not have to be constructed and stored but can be built on demand for the rock volume of immediate interest and specified for a precise task. An underlying well-organised repository of verified hard input data is more important than the models themselves, which are in many ways 'disposable' and built for a specific task.

## 7 Conclusions

- Implicit geological modelling has been shown to be a viable option for the construction of national-scale (in the UK context) volumetric geological models.
- The British Isles have a long and complex geological history, but breaking it into its constituent unconformity-bound storeys creates a functional working stratigraphy for the purposes of implicit modelling.
- The precise stratigraphic horizons and structural complexity of a model will entirely depend on the purpose of the model.
- 'Clean' input data is fundamental to the implicit modelling process, but importantly implicit modelling can also cope with the fuzziness and noise that is inherent in all subsurface geological datasets.
- The implicit modelling process is largely automated and can work with a minimum of 'phantom points' which accelerates the model building process and maintains them in a state where they can be updated and edited.
- The creation of 3D stratigraphic grids as part of the modelling workflow opens up new possibilities in modelling lithofacies and other properties of the rock matrix and its pore space.

## References

British Geological Survey holds most of the references listed below, and copies may be obtained via the library service subject to copyright legislation (contact libuser@bgs.ac.uk for details). The library catalogue is available at: <u>https://envirolib.apps.nerc.ac.uk/olibcgi</u>.

Allen, D.J. et al., 1997. The physical properties of major aquifers in England and Wales. Technical Report WD/97/34 (Environment Agency R&D Publication 8) (Keyworth, Nottingham: British Geological Survey)

Brewer, J.A. et al., 1983. BIRPS deep seismic reflection studies of the British Caledonides. Nature, 305: 206.

Calcagno, P., Chilès, J.P., Courrioux, G., Guillen, A., 2008. Geological modelling from field data and geological knowledge: Part I. Modelling method coupling 3D potential-field interpolation and geological rules. Physics of the Earth and Planetary Interiors, 171(1): 147-157.

Bloomenthal, J., Wyvill, B., 1990. Interactive techniques for implicit modeling, Proceedings of the 1990 symposium on Interactive 3D graphics. ACM, Snowbird, Utah, USA, pp. 109-116.

Booth, K.A., Booth, S.J., Slater, C., 2012. BGS Geological Cross sections & Quaternary Domains: User Guidance Notes. British Geological Survey Internal Report, OR/10/030. 36pp.

Brenchley, P.J., Rawson, P.F., 2006. The Geology of England and Wales (2nd edn). Geological Society: London, viii+559.

Burke, H. et al., 2014. The London Basin superficial and bedrock LithoFrame 50 Model. Nottingham, UK, British Geological Survey, 27pp. (OR/14/029).

Butler, M., Jamieson, R., 2013. Preliminary interpretation of six regional seismic profiles across onshore basins of England. UK Onshore Geophysical Library.

Cameron, T.D.J. et al., 1992. The geology of the southern North Sea. United Kingdom Offshore Regional Report, HMSO, London.

Chadwick, R.A., Holliday, D.W., Holloway, S., Hulbert, A.G., 1995. The structure and evolution of the Northumberland-Solway Basin and adjacent areas. HMSO. .

Cogné, N., Doepke, D., Chew, D., Stuart, F.M., Mark, C., 2016. Measuring plume-related exhumation of the British Isles in Early Cenozoic times. Earth and Planetary Science Letters, 456: 1-15.

Cowan, J., 2016. How to Take Advantage of Geological Bias. <u>http://www.orefind.com/blog/orefind\_blog/2016/05/06/how-to-take-advantage-of-geological-bias</u>.

- Dearman, W.R. et al., 2011. Engineering geology (superficial) map of the United Kingdom. 1:1 000 000. British Geological Survey.
- Evile, L., 2018. Structural Uncertainties in SKUA <u>http://pdgm.custhelp.com/ci/fattach/get/170281/1480420284/redirect/1/filename/Tips\_Tricks\_Structural\_Uncertainties</u> <u>English.pdf.</u>
- Hallam, A., Wignall, P.B., 1999. Mass extinctions and sea-level changes. Earth-Science Reviews, 48(4): 217-250.
- Hibsch, C. et al., 1993. Paleostress evolution in Great Britain from Permian to Cenozoic: a microtectonic approach to the geodynamic evolution of the southern UK basins. Bulletin - Centre de Recherches Exploration-Production Elf-Aquitaine, 17(2): 303-330.
- Janszen, A., Moreau, J., Moscariello, A., Ehlers, J., Kröger, J., 2013. Time-transgressive tunnel-valley infill revealed by a threedimensional sedimentary model, Hamburg, north-west Germany. Sedimentology, 60(3): 693-719.
- Kearsey, T. et al., 2015. Testing the application and limitation of stochastic simulations to predict the lithology of glacial and fluvial deposits in Central Glasgow, UK. Engineering Geology, 187: 98-112.
- Kirby, G.A. et al., 2000. The Structure and Evolution of the Craven Basin and adjacent areas. Subsurface Memoir of the British Geological Survey.
- Kroner, U., Romer, R.L., 2013. Two plates Many subduction zones: The Variscan orogeny reconsidered. Gondwana Research, 24(1): 298-329.
- Laurent, G., 2016. Iterative Thickness Regularization of Stratigraphic Layers in Discrete Implicit Modeling. Mathematical Geosciences, 48(7): 811-833.
- Lawley, R., Garcia-Bajo, M., 2010. The National Superficial Deposit Thickness Model (SDTM V5): A User Guide. British Geological Survey Internal Report, OR/09/049. 18pp.
- Łuszczak, K., Persano, C., Stuart, F.M., 2018. Early Cenozoic Denudation of Central West Britain in Response to Transient and Permanent Uplift Above a Mantle Plume. Tectonics, 37(3): 914-934.
- Mallet, J.-L., 2004. Space-Time Mathematical Framework for Sedimentary Geology. Mathematical Geology, 36(1): 1-32.
- Mathers, S.J. et al., 2014. A geological model of London and the Thames Valley, southeast England. Proceedings of the Geologists' Association, 125(4): 373-382.
- Mckerrow, W.S., Mac Niocaill, C., Dewey, J.F., 2000. The Caledonian Orogeny redefined. Journal of the Geological Society, 157(6): 1149-1154.
- McMahon, N.A., Turner, J., 1998. The documentation of a latest Jurassic-earliest Cretaceous uplift throughout southern England and adjacent offshore areas. Geological Society, London, Special Publications, 133(1): 215-240.
- Newell, A.J., 2018. Rifts, rivers and climate recovery: A new model for the Triassic of England. Proceedings of the Geologists' Association, 129(3): 352-371.
- Newell, A.J., Butcher, A.S., Ward, R.S., 2016. A 3D geological model of post Carboniferous strata in the south Fylde area of the West Lancashire Basin, Blackpool, UK. Nottingham, UK, British Geological Survey, 26pp. (OR/16/007) (Unpublished).
- Newell, A.J., Evans, D.J., 2011. Timing of basin inversion on the Isle of Wight: New evidence from geophysical log correlation, seismic sections and lateral facies change in the Palaeogene Headon Hill Formation. Proceedings of the Geologists' Association, 122(5): 868-882.
- Newell, A.J. et al., 2015a. Fluvial response to Late Pleistocene and Holocene environmental change in a Thames chalkland headwater: the Lambourn of southern England. Proceedings of the Geologists' Association, 126(6): 683-697.
- Newell, A.J., Ward, R.S., Fellgett, M.W., 2015b. A preliminary 3D model of post-Permian bedrock geology in the Vale of Pickering, North Yorkshire, UK. Nottingham, UK, British Geological Survey, 23pp. (OR/15/068) (Unpublished).
- Newell, A.J., Woods, M.A., Farrant, A.R., Smith, H., Haslam, R.B., 2018. Chalk thickness trends and the role of tectonic processes in the Upper Cretaceous of southern England. Proceedings of the Geologists' Association, 129(5): 610-628.
- Paradigm, 2015. SKUA-GOCAD<sup>™</sup> Integrated Earth Modeling. <u>http://www.pdgm.com/resource-library/brochures/skua-gocad/skua-gocad/</u>.
- Parrish, R.R., Parrish, C.M., Lasalle, S., 2018. Vein calcite dating reveals Pyrenean orogen as cause of Paleogene deformation in southern England. Journal of the Geological Society, 175(3): 425-442.
- Peacock, D., 2009. A review of Alpine deformation and stresses in southern England. Italian Journal of Geosciences, 128(2): 307-316.
- Pharaoh, T.C., Morris, J., Long, C.B., Ryan, P.D., 1996. The Tectonic Map of Britain, Ireland and adjacent areas. Sheet 1. 1:1 500 000 Scale. British Geological Survey and Geological Survey of Ireland.
- Pharaoh, T.C. et al., 2011. Structure and evolution of the East Midlands region of the Pennine Basin. Subsurface memoir of the British Geological Survey.
- Poppelreiter, M., Garcia-Carballido, C., Kraaijveld, M., 2010. Borehole image log technology: application across the exploration and production life cycle.
- Reid, R., 2007. Implicit Modelling disasters in the making Part 1. <u>https://www.linkedin.com/pulse/implicit-modelling-disasters-making-part-1-ron-reid/</u>.
- Ringrose, P., Bentley, M., 2015. Reservoir Model Design: A Practitioner's Guide. Springer, Dordrecht, 249 pp.
- Sloss, L., 1963. Sequences in the cratonic interior of North America. Geological Society of America Bulletin, 74(2): 93-114.
- Smith, N.J.P., Kirby, G.A., Pharaoh, T.C., 2005. Structure and evolution of the south-west Pennine Basin and adjacent area. Subsurface memoir of the British Geological Survey.
- Soper, N.J., Woodcock, N.H., 2003. The lost Lower Old Red Sandstone of England and Wales: a record of post-Iapetan flexure or Early Devonian transtension? Geological Magazine, 140(6): 627-647.
- Taylor, G.K., 2007. Pluton shapes in the Cornubian Batholith: new perspectives from gravity modelling. Journal of the Geological Society, 164(3): 525-528.
- Tiley, R., White, N., Al-Kindi, S., 2004. Linking Paleogene denudation and magmatic underplating beneath the British Isles. Geological Magazine, 141(3): 345-351.
- Trewin, N.H., 2002. The Geology of Scotland. Geological Society of London.
- Underhill, J.R., Monaghan, A.A., Browne, M.A.E., 2008. Controls on structural styles, basin development and petroleum prospectivity in the Midland Valley of Scotland. Marine and Petroleum Geology, 25(10): 1000-1022.

Waters, C.N. et al., 2007. Stratigraphical Chart of the United Kingdom:Northern Britain. British Geological Survey, 1 poster. Waters, C.N. et al., 2008. Stratigraphical Chart of the United Kingdom: Southern Britain. British Geological Survey, 1 poster. . Waters, C.N., Terrington, R., Cooper, M.R., Raine, R.B., Thorpe, S., 2015. The construction of a bedrock geology model for the

UK: UK3D\_v2015. British Geological Survey Report, OR/15/069 22pp.
Wellmann, F., Caumon, G., 2018. Chapter One - 3-D Structural geological models: Concepts, methods, and uncertainties. In: C. Schmelzbach (Ed.), Advances in Geophysics. Elsevier, pp. 1-121.