The long-term ecology and evolution of marine reptiles in a Jurassic seaway

Citation for published version:
Foffa, D, Young, MT, Stubbs, TL, Dexter, K & Brusatte, S 2018, 'The long-term ecology and evolution of marine reptiles in a Jurassic seaway' Nature Ecology & Evolution. DOI: 10.1038/s41559-018-0656-6

Digital Object Identifier (DOI):
10.1038/s41559-018-0656-6

Link:
Link to publication record in Edinburgh Research Explorer

Document Version:
Peer reviewed version

Published In:
Nature Ecology & Evolution

Publisher Rights Statement:
Copyright © 2018, Springer Nature

General rights
Copyright for the publications made accessible via the Edinburgh Research Explorer is retained by the author(s) and / or other copyright owners and it is a condition of accessing these publications that users recognise and abide by the legal requirements associated with these rights.

Take down policy
The University of Edinburgh has made every reasonable effort to ensure that Edinburgh Research Explorer content complies with UK legislation. If you believe that the public display of this file breaches copyright please contact openaccess@ed.ac.uk providing details, and we will remove access to the work immediately and investigate your claim.
The long-term ecology and evolution of marine reptiles in a Jurassic seaway

Davide Foffa\textsuperscript{a,*}, Mark T. Young\textsuperscript{a}, Thomas L. Stubbs\textsuperscript{b}, Kyle G. Dexter\textsuperscript{a}, Stephen L. Brusatte\textsuperscript{a}

\textsuperscript{a}School of GeoSciences, University of Edinburgh, Grant Institute, James Hutton Road, Edinburgh, Scotland EH9 3FE, United Kingdom; \textsuperscript{b}School of Earth Sciences, University of Bristol, Life Sciences Building, 24 Tyndall Avenue, Bristol BS8 1TQ, England, United Kingdom.

*corresponding author
Marine reptiles flourished in the Mesozoic oceans, filling ecological roles today dominated by crocodylians, large fish, sharks, and cetaceans. Many groups of these reptiles coexisted for over 50 million years, through major environmental changes. Little is known, however, about how the structure of their ecosystems or their ecologies changed over millions of years. We use the most common marine reptile fossils—teeth—to establish a quantitative system that assigns species to dietary guilds, and then track the evolution of these guilds over the ca. 18 million year history of a single seaway, the Jurassic Sub-Boreal Seaway of the United Kingdom. Groups did not significantly overlap in guild space, indicating that dietary niche partitioning enabled many species to live together. Although a highly diverse fauna was present throughout the history of the seaway, fish and squid-eaters with piercing teeth declined over time while hard-object and large-prey specialists diversified, in concert with rising sea-levels. High niche partitioning and spatial variation in dietary ecology related to sea depth also characterize modern marine tetrapod faunas, indicating a conserved ecological structure of the world’s oceans that has persisted for over 150 million years.
During the Mesozoic Era, when dinosaurs ruled the land, the oceans were teeming with a diversity of large reptiles adapted to an aquatic lifestyle. These included iconic groups such as the long-necked plesiosauroiids, big-headed pliosauroiids, dolphin-like ichthyosauriids, and an aberrant assemblage of crocodile relatives called thalattosuchians (subdivided into the gharial-like teleosauriids and cetacean-like metriorhynchiids). These groups were exceptionally diverse and coexisted in the same environments for over 50 million years, from the Early Jurassic (ca. 180 million years ago) to the Early Cretaceous (ca. 130 million years ago), through major changes in sea-level, climate, and ocean chemistry. They formed complex ecosystems and filled a variety of ecological roles—ranging from fast-swimming fish-eaters to large-bodied apex predators—that are today dominated by crocodylians (in near-shore environments), sharks and other large fishes, and marine mammals. As modern oceans are undergoing rapid changes, understanding Mesozoic marine reptile ecosystems may provide critical insight into how species at or near the top of the food chain might respond to environmental shifts.

Although the phylogenetic relationships and taxonomic diversity patterns of Mesozoic marine reptiles have been the subject of intensive focus, much less is known about their ecology, about the structure of their ecosystems, and how their ecosystems changed over millions of years of evolutionary time. Two main problems have hindered progress. First, it is difficult to determine the ecological niches and feeding styles of extinct species, particularly when they are represented by limited fossil material. The pioneering work of Massare assigned marine reptiles to broad ecological guilds, but these are qualitative in nature and have not been universally accepted. Second, the marine reptile fossil record is notoriously patchy, dominated by fossil-rich localities (Lagerstätten) that register snapshots of ecosystems but do not document long-term changes. These issues hamper comparisons
between Mesozoic and modern marine faunas, and make it difficult to draw parallels between
the fossil record and contemporary environmental change.

Here, we use teeth—the most common marine reptile fossils, which are often
preserved in the absence of more complete skeletal remains—to evaluate feeding ecology.
Our quantitative approach validates the guild system of Massare, and allows species to be
placed in a functional morphospace that reflects the breadth of dietary niches. We then track
changes in how these niches were filled over time, focusing on the remarkable fossil record
of the Jurassic Sub-Boreal Seaway of the United Kingdom. Marine reptiles have long been
known from two Lagerstätten formed in this seaway, the Oxford Clay Formation (Callovian-
early Oxfordian, ~165-161 Ma) and the Kimmeridge Clay Formation (Kimmeridgian-early
Tithonian, ~157-148 Ma), but recent work has clarified the fossil record of the
intervening Corallian Group (~161.5-157.3 Ma). Thus, we can now examine long-term
ecological changes in a single seaway spanning ca. 18 million years of the Middle-Late
Jurassic, a time of known environmental changes that began with recovery from a drop in
sea-level linked to a major glaciation, followed by a gradual rise in sea-level that culminated
in a chaotic interval of rapid shifts in water depth.

Results
Principal Coordinates Analysis (PCO) of our dental morphology dataset ordinated all
specimens into a morphospace, the first three axes of which describe over 63% of total
variance (Fig. 1; Supplementary Figures 2-3; Supplementary Table 1). A linear discriminant
analysis found that clusters of species in the morphospace correspond to the feeding guilds of
Massare, originally qualitatively defined based on comparisons of tooth shape, wear, and
size and with modern marine tetrapods (Supplementary Table 6). When the 35 specimens in
our dataset (encompassing 25 taxa) that were also included in Massare’s study were assigned to Massare’s guilds \textit{a priori}, a jackknifing procedure found that our PCO axes successfully discriminated these groups, with 84\% of species correctly attributed to the guild Massare assigned them to. This supports broad correspondence between our PCO morphospace and Massare’s guilds, but 16\% of species are mis-attributed, which may be because some species previously known from limited fossil material (particularly metriorhynchids) were misclassified when Massare introduced the guilds. We therefore used our PCO results to establish a revised system of five guilds, which linear discriminant analysis finds to be 97.30\% accurate. Along with the fact that characters in our dataset were chosen to represent functionally significant features related to feeding, this indicates that the PCO morphospace can be interpreted as a functional morphospace reflecting diet (Table 1). This link was previously demonstrated by Massare\textsuperscript{7}, by assessing tooth morphology, shape and gut contents of the same species, and validated with comparisons with modern marine tetrapods (for which dietary data are available).

<table>
<thead>
<tr>
<th>Guild</th>
<th>Apex shape</th>
<th>Ornamentation</th>
<th>Cutting edges</th>
<th>Tooth size and shape</th>
<th>Examples</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cut</td>
<td>Pointed</td>
<td>Normally largely absent (in geosaurines, except cf. ‘Metriorhynchus’ hastifer)</td>
<td>Two functional cutting edges always present</td>
<td>Very large: generally &gt; 4cm. Robust crowns, mid-to-high CR*</td>
<td>Dakosaurus, Plesiosuchus, Geosaurus, cf. ‘Metriorhynchus’ hastifer</td>
</tr>
<tr>
<td>Generalist-Cut</td>
<td>Pointed</td>
<td>Present: high-relief with serration morphologies</td>
<td>Two or more cutting edges always present</td>
<td>Very large: generally &gt; 5cm. Robust crowns, mid-to-high CR*</td>
<td>Pliosaurus spp.</td>
</tr>
<tr>
<td>Generalist-Pierce</td>
<td>Pointed</td>
<td>Variable, it may be high relief</td>
<td>None, or non-prominent. If present they are smooth and non-serrated</td>
<td>Variably large: generally &gt; 5cm. Normally conical. Variable CBR.</td>
<td>Liopleurodon, Simolestes, ‘Pliosaurus’ andrewsi</td>
</tr>
</tbody>
</table>
**Table 1.** Description of the main tooth features diagnosing the five guilds as used in this study. Note that this is a key that can be used to assign specimens to guilds based on consideration of a few general features, but more rigorous assignment can be made numerically using Linear Discriminant Analysis of PCO scores. Taxa in bold are classified in a different guild compared to Massare’s System (see Supplementary Table 7, Appendix S3, S4). The table is adjusted from Massare (1987). *CR: Crown height to base Ratio.

<table>
<thead>
<tr>
<th>Guild</th>
<th>Shape</th>
<th>Ornamentation</th>
<th>Adjacent Region of Morphospace</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pierce</td>
<td>Pointed</td>
<td>Variable, but never high relief</td>
<td>None, or non-prominent. In metriorhynchin es if they are present they are smooth, or not functionally serrated. Normally small (&lt;3 cm), but can be large ( &gt; 3 cm). Mid-to-high CR*, lateral compression variable (weak or absent, in plesiosauroids and metriorhynchines; laterally compressed in geosaurines).</td>
</tr>
<tr>
<td>Smash</td>
<td>Pointed to Rounded</td>
<td>NA</td>
<td>None</td>
</tr>
<tr>
<td>Crunch</td>
<td>Rounded</td>
<td>Strongly ornamented, with high-relief ridges and may have serration morphologies</td>
<td>Prominent carinae only on the top half of the crown. Robust and conical, poorly to non-laterally compressed. Mid-to-low CR*.</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Many thalattosuchians (teleosaurids and metriorhynchids), plesiosauroids, and small-bodied pliosaurids cluster together in morphospace, due to their thin teeth that lack serrations (Pierce Guild), similar to modern shallow-water river dolphins and gharials; they are inferred to be fish and squid-eaters (Fig. 1, Table 1). An adjacent region of morphospace is occupied by the soft prey-eating Smash Guild, which is almost exclusively filled by ichthyosaurs with conical, non-carinated and non-serrated teeth (Fig. 1, Table 1). Strongly ornamented, blunt crowns of machimosaurin teleosaurids and the geosaurine Torvoneustes belong to the Crunch Guild, inferred as hard-object (e.g. sea turtles) feeders (durophages) (Fig. 1, Table 1). There are two clusters of cutting-type dentitions that correspond to different types of macrophagy (feeding on large-bodied prey), analogous to modern deep-water cetaceans like killer whales: the Cut Guild of geosaurine metriorhynchids (Geosaurus, Plesiosuchus, and Dakosaurus) with large and serrated teeth, and the Generalist-Cut Sub-Guild (the macrophagous partition
of the Generalist Guild) of pliosaurids with huge, robust, heavily ornamented teeth. The Generalist-Pierce Sub-Guild (the other partition of the Generalist Guild), characterised by large, conical and variably ornamented teeth and mostly including large Callovian pliosaurids, fills a space between the Generalist-Cut and Pierce Guilds (Fig. 1, Table 1).

We assessed changes in the dietary ecology of marine reptiles during the ca. 18 million year history of the Sub-Boreal Seaway by testing for changes in morphospace overlap and morphological disparity (amount of occupied morphospace) between phylogenetic groups. The major marine reptile groups do not significantly overlap in morphospace overall, and within each time slice (Appendix S2), indicative of large-scale dietary niche partitioning, but also a likely phylogenetic signal (e.g. through shared evolutionary ancestry). However, individual groups show evidence of morphospace migration over time (Fig. 2). Pliosaurids are the most extreme example, as they make a (nearly) significant jump (Supplementary Table 2) between their scattered Callovian morphospace into a more restricted region in the ensuing Oxfordian. This change is followed by another significant shift between the Oxfordian and Kimmeridgian, as a consequence of the appearance of the genus *Pliosaurus*.

Other groups do not exhibit significant shifts between successive time intervals, but do show significant changes between end points (e.g., Callovian vs. Tithonian, or Oxford Clay vs. Kimmeridge Clay Formations), which is indicative of gradual ecological changes.

There are no significant differences over time in the disparity of the pooled sample of all marine reptile groups in the morphospace (as shown by permutation tests on range and variance measures of morphospace occupation), indicating that an ecologically diverse fauna persisted throughout the entire history of the seaway (Supplementary Table 5). There are few instances of significant disparity changes within individual groups across successive time intervals, despite turnover at the species level (Fig. 2). Metriorhynchid groups are the
exceptions, as geosaurines significantly increased in disparity from the Oxfordian to the Kimmeridgian, as their variety of niches expanded, in concert with the decline of fish-eating metriorhynchines. This implies that, although groups were migrating through morphospace over time, most continued to fill a similar breadth of niches, albeit in different regions of the morphospace (Fig. 2). Partial disparity trends show that teleosaurids and metriorhynchids make up a large proportion of overall disparity in the Callovian but decline over time, whereas geosaurines and macrophagous pliosaurids (*Pliosaurus*) become relatively more disparate (Fig. 3). When partial disparity is instead tracked by guild, Pierce taxa are highly disparate early but decline into the Oxfordian and beyond, as Crunch, Smash, and Cut species assume a larger share of overall disparity (Fig. 3).

These quantitative tests allow us to identify several major trends. Pliosaurids were diverse in the Callovian, ranging across a broad span of fish-eating Pierce and apex-predator Generalist/Generalist-Pierce guilds, but then in the Oxfordian atrophied into a more restricted region of macrophagous morphospace (Generalist/Generalist Cut), where they diversified further in the Kimmeridgian, without migrating back into the Pierce Guild. Similarly, teleosaurids were highly diverse in the Callovian, including long-snouted fish-eaters in the Pierce Guild and durophages in the Crunch Guild, but the former species mostly disappeared from the Oxfordian onwards while the hard-object feeders persisted. Geosaurines began with a large diversity of taxa spanning the Pierce Guild in the Callovian, and in the Oxfordian bifurcated into a Crunch group that approached the durophagous teleosaurids in morphospace and a Cut group of large-prey specialists, which were distinct from the macrophagous Generalist-Cut pliosaurids in morphospace. Metriorhynchines included several Pierce Guild piscivores in the Callovian, but then mostly disappeared afterwards. Ichthyosaurs were relatively stable in almost exclusively occupying the soft-prey-eating Smash Guild from the Callovian to Tithonian, but their share of partial disparity increases over time. Sample sizes
for plesiosauroids are too small to reasonably interpret, although they seem to stably occupy the Pierce Guild through time.

**Discussion**

In agreement with previous studies\(^5,7,15\), we argue that there is a tight link between tooth morphology and dietary ecology in Jurassic marine reptiles. By assessing a limited number of discrete features and measurements of the teeth, species can be placed in a functional morphospace that distinguishes ecological guilds (Fig. 1). This morphospace differentiates marine reptiles that fed in different ways, including soft-object feeders, piercers of fish and squid, durophagous hard-object crushers, and apex predator macrophages that specialized on large vertebrate prey\(^5,7,15\). Our approach is a powerful tool for predicting the feeding habits of long-extinct species, as it focuses on the most commonly preserved marine reptile fossils (teeth), and can incorporate even minimally complete specimens. Our approach provides a quantitative method for projecting Massare’s guilds\(^7\)—which have long been used by marine reptile workers—into a numerically-derived morphospace, meaning specimens can be assigned to these guilds more objectively, and changes in guild occupation over time can be analysed statistically.

Our study reveals the ecological structure of marine reptile faunas in the Sub-Boreal Seaway during ca. 18 million years of the Middle-Late Jurassic. The positions of species in our functional morphospace give insight into niche occupation. The major marine reptile groups do not significantly overlap with each other in morphospace, meaning that different groups generally employed distinct dietary strategies (possibly in part due to shared evolutionary ancestry). Partitioning niches in this way may explain why such a great diversity of marine reptiles were able to coexist in the Mesozoic oceans\(^13\), and parallels the situation in modern oceans, where aquatic tetrapods subdivide ecological space by feeding in different
ways and on different prey. Evidently, Jurassic marine reptiles partitioned niches to a fine
degree, as testified by the development of two distinct and coexisting forms of macrophyg:
the robust-toothed pliosaurids in the Generalist-Cut Guild and the thinner, slicing-toothed
geosaurines of the Cut Guild. Other groups converged on similar niches—most notably
machimosaurin teleosaurids and *Torvoneustes*-lineage geosaurines that independently
colonized the same durophagous area of morphospace—which speaks to the maintenance of
key niches over long spans of time. We also find no significant differences in overall
morphological disparity of the Sub-Boreal assemblages over time, illustrating that a diverse
marine reptile fauna was present throughout the entire history of the seaway, and in general
terms was resilient to environmental change.

Nonetheless, the shifting distribution of species in the morphospace over time does
provide evidence for long-term ecological changes. Although the imprecise ages of fossils
make it difficult to untangle the tempo of these changes, they appear to be a mix of sudden
transformations at or near the Callovian-Oxfordian (Middle-Late Jurassic) boundary and
more gradual changes that occurred throughout the Oxfordian, Kimmeridgian, and Tithonian,
as sea-levels rose and water depth increased. Most severe was the decimation of the Pierce
Guild, which was filled by a diversity of teleosaurids, metriorhynchines, and small-bodied
pliosaurids in the Callovian, but was then largely vacated from the Oxfordian onwards.
Essentially, this reflects a drastic decline of nearshore, piscivorous species. Metriorhynchines
excelled in this niche and were the most abundant component of the Callovian Oxford Clay
ecosystem, but are almost unknown from the later Kimmeridge Clay. Replacing the Pierce
species was a greater variety of macrophagous taxa, particularly large pliosaurids and
geosaurines, and durophages, including the specialized machimosaurin lineage of
teleosaurids. At the same time, ichthyosaurs maintained their position in the Smash Guild and
diversified further, reflecting a blossoming of deep-diving species that fed on similar prey to
We hypothesize that these large-scale changes in marine reptile functional diversity and niche occupation in the Jurassic Sub-Boreal Seaway were related to changes in water depth over time, analogous to how modern aquatic tetrapod diversity and ecology are known to change from shallow water (nearshore) to deeper water (offshore) habitats. It is well established that the Sub-Boreal Seaway became generally deeper as global sea-levels rose from the Callovian into the Oxfordian, and then across the Oxfordian, Kimmeridgian, and early Tithonian. The main fossiliferous beds of the Callovian Oxford Clay Formation were deposited in nearshore waters ca. 50 metres deep; the middle-late Oxfordian Corallian Group rocks formed in deeper waters during a time of warming and sea-level transgression; and the main fossil-bearing units of the Kimmeridge Clay Formation, spanning the Kimmeridgian-Tithonian boundary, were deposited on continental shelves 100-200 metres deep. Although numerous factors (ranging from water temperature and turbidity to productivity and seasonality) control the distribution of extant marine tetrapods and their prey, water depth is widely recognized as one of the key drivers of ecological partitioning. While small delphinoids such as bottlenose and spotted dolphins can be found both nearshore and sometimes further shelf-ward, large delphinoids like killer whales predominately live in deeper, open waters and infrequently venture nearshore, and their abundance on continental shelves increases with water depth. The diets of mid-shelf to offshore delphinoids also becomes increasingly dominated by larger prey, and only off-shelf species actively prey upon large tetrapods.

In the Jurassic Sub-Boreal Seaway, a variety of marine reptiles shared environments by feeding in different ways, and nearshore fish-eating marine reptiles declined and open-ocean macrophages and durophages proliferated as sea-level increased over millions of years of evolutionary time. In the modern oceans, numerous species of large vertebrates coexist by
partitioning dietary niches, and there is a noted ecological partitioning of shallow-water
small-object feeders and deep-water, large-prey specialists. These parallels between Jurassic
and modern oceans—separated in time by ca. 150 million years, occupied by different groups
of species, and shaped by vastly distinct paleogeography, temperature, and ocean chemistry—
may indicate a conserved ecological structure near the top of ocean food webs over time.

Methods

Dataset. We compiled a dataset of 22 functionally-relevant anatomical characteristics of the
teeth scored for 122 specimens of marine reptiles (representing ~50 species) that lived in the
Jurassic Sub-Boreal Seaway of the modern-day United Kingdom during the Callovian-
Tithonian stages of the Jurassic (Appendix S1). The specimens come from a variety of
localities and lithological facies within the Jurassic Sub Boreal Seaway basins21. It is possible
that the lower number of Oxfordian specimens is related to preservation (or sampling) bias of
the Corallian Group facies compared to the fossil-rich and better exposed Oxford Clay
Formation and Kimmeridge Clay Formation21. However, by focusing on the most commonly
collected and preserved fossils (teeth), we minimize these biases. We focused on dental
morphology for the following reasons: 1) teeth are more commonly preserved as fossils than
any other part of the marine reptile skeleton; 2) teeth were the primary source of information
that Massare7 used to assign marine reptiles into feeding guilds; 3) multivariate analyses of
tooth measurements, of the type encapsulated in our dataset, have been commonly applied to
other reptile groups (most notably dinosaurs41,42) to determine feeding habits and track long-
term trends in palaeoecology.

Included in our dataset are teeth belonging to the three major marine reptile clades
that lived in the Sub-Boreal Seaway—Plesiosauria, Ichthyosauria, and Thalattosuchia—and
all major subclades within these lineages. We designed our specimen sampling to maximise the number of complete specimens for each taxon in each time bin. We selected an approximately equal number of specimens for each taxon to avoid oversampling biases. All tooth crowns in our dataset are from the anterior part of the tooth row, to avoid inflation of diversity caused by the marked heterodonty of some taxa\textsuperscript{15,43,44}. Selecting the largest teeth does not constitute a major problem in the interpretation of the final results because the signal in the analyses is dominated by the discrete characters, which code features that do not significantly change along the tooth row. Additionally, the largest ‘fangs’ are those that undergo the largest stress during predation, and thus are ideal for investigating feeding ecology\textsuperscript{7,43,44}. It is also worth noting that disarticulated teeth cannot always be oriented in their correct mesiodistal orientation, so the distinction between upper or lower jaw teeth is unnecessary.

Each specimen was scored for the 5 continuous and 17 discrete characters in our dataset (Appendix S1), which were selected largely from published phylogenetic and functional datasets\textsuperscript{12,18,19,45,46}. The main sources for discrete characters were the analyses of Young et al. (2016)\textsuperscript{46}, Foffa et al. (2017)\textsuperscript{45}, and Fischer et al. (2015, 2016, 2017)\textsuperscript{12,18,19}; as these studies were designed for specific lineages, it was necessary to modify the definitions and states of some characters, to make them broadly applicable to all marine reptiles. The modified characters were specifically targeted to describe tooth shape, proportions, ornamentation, and cutting edge (carina and denticle) morphologies (Table 1, 2) (Supplementary Figure 1). Most continuous measurements were taken directly from specimens with digital callipers, except for the curvature and crown angles (C4 and C5) that were measured using ImageJ\textsuperscript{47}, and a small number that were taken from the literature (Supplementary Information, Supplementary Figure 1).

<table>
<thead>
<tr>
<th>General aspect</th>
<th>Carinae and serrations</th>
<th>Ornamentation</th>
<th>Roots</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1.</td>
<td>Apicobasal crown height – CH</td>
<td></td>
<td></td>
</tr>
<tr>
<td>D1.</td>
<td>Crown mediolateral compression</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C2.</td>
<td>Crown ratio – CR</td>
<td></td>
<td></td>
</tr>
<tr>
<td>D12.</td>
<td>Crown cross-section</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C3.</td>
<td>Crown base ratio – CBR</td>
<td></td>
<td></td>
</tr>
<tr>
<td>D13.</td>
<td>Trifaceted labial side</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C4.</td>
<td>Labial-Lingual curvature – LLcufrv</td>
<td></td>
<td></td>
</tr>
<tr>
<td>D15.</td>
<td>Tooth crown apex – shape</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C5.</td>
<td>Crown Angle – Cang</td>
<td></td>
<td></td>
</tr>
<tr>
<td>D16.</td>
<td>Root cross-section</td>
<td></td>
<td></td>
</tr>
<tr>
<td>D7.</td>
<td>Enamel surface ornamentation: anastomosed pattern</td>
<td></td>
<td></td>
</tr>
<tr>
<td>D8.</td>
<td>Enamel ornamentation presence and density: lingual side</td>
<td></td>
<td></td>
</tr>
<tr>
<td>D9.</td>
<td>Enamel ornamentation presence and density: labial side</td>
<td></td>
<td></td>
</tr>
<tr>
<td>D10.</td>
<td>Enamel ridges, relief</td>
<td></td>
<td></td>
</tr>
<tr>
<td>D11.</td>
<td>Ornamentation interfering with the carinae or cutting edges – false denticles</td>
<td></td>
<td></td>
</tr>
<tr>
<td>D14.</td>
<td>Enamel texture</td>
<td></td>
<td></td>
</tr>
<tr>
<td>D17.</td>
<td>Bulbous root larger than the crown</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 2. Table of continuous (C) and discrete (D) morphological characters used to represent marine reptile dentitions. See Supplementary Information for extended descriptions of each character.

**Multivariate analysis.** The continuous characters were standardised using z-transformation (distributions were equalized to the same mean value, \( \mu = 0 \), and standard deviation, \( \sigma = 1 \))\(^{11,48} \). The entire taxon-character matrix (Appendix S1) was then transformed into a Gower distance matrix (necessary for the combination of ordered discrete and continuous characters)\(^{49} \) and subjected to Principal Coordinates Analysis (PCO) in PAST v.3 and R v3.4.3\(^{50,51} \), following the procedure in Stubbs and Benton (2015)\(^{11} \). The small number of missing values (8.2% of the total scores) were automatically accounted for by pairwise deletion. The scores of the first three PCO axes (which describe 28.54%, 22.16%, and 12.43% of total variance, respectively: Supplementary Table 1) were used to generate morphospaces for data visualization (Figs. 1-2, Supplementary Figures 1-2), and the 15 PCO axes that accounted for at least 0.5% of total variance were retained for discriminant function analysis, statistical tests of morphospace overlap, and disparity calculations.

We ran a Linear Discriminant Analysis (LDA) (Appendix S3) to test the ability of the...
PCO scores to assign individuals to the feeding guild assignments of Massare. The 35 specimens in our dataset that were also included in Massare’s study were a priori assigned to the guilds that Massare originally assigned them to (four guilds total: Pierce [also tested for separate Pierce I and Pierce II], Crunch, Smash, Cut) (for more details see the LDA Guild Sensitivity Analyses in Appendix S4), and the percentages of correct specimen-guild matches were determined using a jackknifing test in PAST v.3 (see Supplementary Information, Appendix S3). This revealed that 84% of specimens were correctly assigned to the Massare’s original guilds (the same percentage, 84%, if the Pierce I and II guilds of Massare are split into two), indicating a broad correspondence between our quantitative PCO morphospace and Massare’s qualitative guilds (see Supplementary Information, Appendix S3, S4).

New fossil discoveries and reanalyses of key specimens suggest that some of the guild assignments of Massare may be problematic, perhaps explaining why 16% of specimens are incorrectly assigned by the LDA. Over the last few decades, many specimens used in Massare’s study have been re-evaluated (particularly metriorhynchids) and further details of tooth morphology have been described (particularly regarding carinae and denticles) (Appendix S3). Thus, we used the results of our PCO analysis—particularly the visual spread of taxa in morphospace—to modify Massare’s guilds into a new system of five guilds: Pierce, Crunch, Smash, Cut, and Generalist (subdivided into Generalist-Pierce, and Generalist-Cut) (Appendix S3, S4). We assigned the same 35 specimens from taxa shared with Massare’s study to one of these guilds a priori, and then ran a second LDA, which correctly attributes 97.3% of the specimens to the proper guild. This indicates that our morphospace can be used to sensibly cluster species into guilds, and thus be interpreted as a dietary function space. This second LDA also serves to classify each of our 122 specimens into its best-fit guild. The regions of our PCO morphospace occupied by each guild are denoted in Figure 1. This is the first attempt to project Massare’s qualitative guilds into a numerically-derived morphospace.
Note that in creating our revised guild system, we preferred a unified Pierce guild over Massare’s original subdivision of Pierce I and Pierce II guilds, because this distinction relied on wear patterns and features of cranial morphology that are not captured in our dataset (but see Appendix S4 for sensitivity analyses).

**Statistical analyses.** Specimens were binned by clade, guild, and time in order to conduct statistical analyses of morphospace overlap and morphological disparity.

We employed a hierarchy of taxonomic bins. We broadly divided the specimens into the three main order-level clades: Plesiosauria, Ichthyosauria, and Thalattosuchia. We then ran additional analyses in which these large clades were subdivided into less inclusive monophyletic groups of family-level, and subfamily-level. Plesiosauria was subdivided into Plesiosauroida and Pliosauridae. Thalattosuchia was split into Metriorhynchidae and Teleosauridae, both of which were further divided (into Metriorhynchidae/Geosaurinae for the former, and into Machimosaurini/non-Machimosaurini for the latter). As all ichthyosaur specimens belong to Ophthalmosauridae, this group was not subdivided. Finally, for the disparity analyses, we examined three further lineages within Pliosauridae (non-Pliosaurus pliosaurs and *Pliosaurus* spp.) and Geosaurinae (the ‘T-clade’: *Tolvoneustes-Metriorhynchus hastifer*-Mr. Passmore’s specimen clade; the ‘GPD clade’: *Plesiosuchus-Dakosaurus-Geosaurus* clade; and ‘Basal Geosaurinae’, which includes ‘Metriorhynchus brachyrhynchus’, with and without *Tyrannoneustes lythrodectikos* – because of the unstable position of the latter in the latest phylogenetic analyses\(^\text{17,45}\)).

We employed four time bins when analysing trends over the Jurassic. These correspond to stage level: Callovian (166.1–163.5 Ma), Oxfordian (163.5–157.3 Ma), Kimmeridgian (157.3–152.1 Ma), and early Tithonian (152.1–148.5 Ma). The average length of these time bins is 4.4 Ma, with a minimum of 2.6 Ma for the Callovian and maximum of 6.2 Ma for the Oxfordian. Given the age uncertainty of several specimens, equal-length bins
were deemed unreasonable because too many specimens would be assigned to multiple time bins, decreasing the power of our analyses. We ran subsidiary analyses in which specimens was also assigned to stratigraphic bins representing the main marine reptile faunas of the Sub-Boreal Jurassic Seaway: Oxford Clay Formation (~Callovian - early Oxfordian), ‘Corallian Group’ (middle - late Oxfordian), and Kimmeridge Clay Formation (Kimmeridgian - early Tithonian). This binning scheme demonstrates changes in a series of temporally successive Lagerstätten. We recognize that, for both binning schemes, each time bin includes a time-averaged sample, as is necessarily the norm in most palaeoecological analyses of long-term change. Thus, these bins do not exactly represent individual ecosystems that existed at a moment in time, but rather summarize the pool of species present during the finest temporal resolution available.

We assessed whether taxonomic groups significantly overlapped in the overall morphospace, and for each time interval, using non-parametric multivariate analysis of variance (NPMANOVA) in R (Appendix S2). The null hypothesis is that there is no difference in the location of group centroids in PCO space; significant deviation from the null indicates that the groups in question occupy significantly different areas of morphospace. The p values were adjusted using the false-discovery rate (FDR) method to account for ‘false discoveries’ error that may be introduced by multiple comparisons. Changes in morphospace occupation over time, if confirmed by NPMANOVA, indicate the migration of clades into different niche space.

We measured the breadth of morphospace occupied by taxa by calculating morphological disparity. We used two metrics to quantify disparity: the sum of variances and the sum of ranges on the PCO axes for each group in question. Variance is a measure of the spread of taxa in morphospace relative to the group centroid, whereas range denotes the overall volume of morphospace occupied by the group. These disparity metrics were
calculated in R using functions in the ‘dispRity’ package\textsuperscript{55} Statistical significance of disparity differences between groups, or within groups across time, were assessed by a permutation test developed by Steve Wang\textsuperscript{56}, which determined whether there was a significant difference in the observed disparity value between the two comparisons and the expected disparity difference between them. As the expected difference is generated based on the size of each group, this procedure accounts for sample size differences between the groups, which otherwise could be a major source of bias (particularly for sum of ranges).

We also tracked partial disparity over time, for taxonomic groups and guilds (Fig. 3). The contribution of each group/guild to overall disparity in each time bin was calculated as the average squared distance of each group/guild member point from the overall time bin centroid, with the resulting value weighted by a factor taking into account the sample size of the group/guild compared to the overall sample\textsuperscript{57}. This procedure was conducted with the Morphological Disparity Analyses (MDA) package for MATLAB\textsuperscript{58}.

**Data availability**

The authors declare that all the data supporting the findings of this study are available within the paper and its supplementary information files. The R-codes used to perform statistical tests are available from the corresponding author upon reasonable request.

**References**


545 Foundation for Statistical Computing, Vienna, Austria. ISBN 3-900051-07-0,
546 URL http://www.R-project.org/
548 and powerful approach to multiple testing. *Journal of the Royal Statistical Society, Series
553 10.5281/zenodo.55646
555 avian body plan culminated in rapid rates of evolution across the dinosaur-bird transition.
556 Current Biology 20: 2386–2392.
558 *Paleobiology* 19: 403–419.

**Acknowledgements**

561 We thank Deborah Hutchinson and Isla Gladstone (BRSMG), Matthew Riley (CAMSM),
562 Paul Tomlinson (DORCM), Neil Clark (GLAHM), Steve Etches (MJML), Lorna Steel
563 (NHMUK), Eliza Howlett and Hilary Ketchum (OUMNH) and Emma Jarvis, Sarah King and
564 Stuart Ogilvy (YORYM) for access and guidance during DF’s visits to museum collections.
565 DF's museum visits were funded by the Small Grant Scheme ‘2015 Wood Award’
566 (PASW201402), the Systematics Research Fund, and the Richard Owen Research Fund by
567 the Palaeontographical Society. MTY and SLB are supported by a Leverhulme Trust
Research Project grant (RPG-2017-167), and SLB is supported by a Marie Curie Career Integration Grant (630652). We thank Paige dePolo for comments on the manuscript, and Mark Puttick and Thomas Guillerme for discussion and technical support. We are grateful the reviewers Dr. Judy Massare, Dr. Benjamin C. Moon for the useful comments that greatly improve the quality of this manuscript.

**Author contributions**

DF led the project, conceived the study and wrote the initial draft manuscript. MTY and SLB helped develop the project, edited drafts, and provided guidance on statistical analyses. SLB wrote the final manuscript, which was revised by all authors. DF designed and performed the analyses with technical support from TLS and KGD.

**Competing interests**

The authors declare no competing interests.

**Figure Captions**

**Figure 1.** Morphospace plots showing the distribution of marine reptile specimens based on tooth morphology. **a.** 3D plot of PCO1-PCO2-PCO3, derived from Principal Coordinates Analysis of our dental dataset; **b.** approximate position of the ‘feeding guilds’ (originally outlined by Massare” and modified here) in the PCO morphospace. Tooth drawings depict the general tooth morphologies of key regions of the morphospace.

**Figure 2.** Morphospace plots showing the distribution of marine reptile clades based on tooth morphology through time, only statistically significant ecological and evolutionary shifts are noted. The morphospaces are 3D plots of PCO1-PCO2-PCO3, derived from Principal Coordinates Analysis (Fig. 1). The radiations and declines of groups through time gradually
changed the morphospace/ecosystem composition and partitioning. Note that some groups
may have been limited to certain parts of ecomorphospace by evolutionary constraints.

Figure 3. Partial disparity of Jurassic Sub-Boreal Seaway marine reptile, mapped against
global sea-level. a. Partial disparity of taxonomic groups, b. Partial disparity of dietary
guilds; c. sea-level curve (modified from Haq 1987)\textsuperscript{30}, with fossil rich-intervals from the Sub-
Boreal Seaway noted.