Discriminating faunal assemblages and their palaeoecology based on museum collections: the Carboniferous Hurlet and Index limestones of western Scotland, UK

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Synopsis

Historic collections of Scottish Carboniferous macrofossils stored at the British Geological Survey (BGS), Edinburgh include the sole remaining sources of palaeontological data from numerous localities. Exploratory numerical analyses of such collections from the Hurlet and Index limestones of Ayrshire compare favourably with published qualitative assessments of faunal assemblages and palaeoenvironments; demonstrating that old collections can still be used in modern palaeoecological investigations. Macrofaunas from these formations comprise mainly brachiopods and molluscs and were collected from 67 localities that yielded 20 and 94 samples from the Hurlet and Index limestones respectively. Limitations of the presence/absence data were partly overcome by consolidation and restriction of aspects of the data set. Seriation indicates the lithological and environmental gradients of taxa. Cluster analysis reveals groups of samples linked to lithofacies. Principal Components Analysis (PCA) of diversity data derived from the data set in terms of

numbers of genera in higher taxa highlights differences in gross taxonomic composition in terms of trophic structure, lithology and environment.

Supplementary material: lists of localities, taxa and sample lithologies used in this study are available at http://www.geolsoc.org.uk/SUP00000.

Introduction

Carboniferous rocks at outcrop underlie much of central Scotland but are predominantly covered by Quaternary deposits, and good exposures of the sedimentary rocks are rare, especially in the economically important coal bearing Namurian and Westphalian successions. However, extensive mining, quarrying and sinking of cored boreholes associated with the exploration and exploitation of coal, ironstone and refractory materials (including limestone) from the late 18th to the mid 20th century yielded a vast amount of detailed palaeontological and stratigraphical knowledge of these rocks (Cameron & Stephenson 1985; Read *et al.* 2002; Trewin & Rollin 2002). Deep mining has ceased but the palaeontological material collected during exploration and exploitation has been retained, often as the sole remaining source of palaeontological data. This is a manifestation of a much wider phenomenon that emphasises the importance of historical palaeontological collections (e.g. see Allmon 2005). The question then arises as to whether these data from the BGS collections are sufficiently complete to render them amenable to palaeoecological analysis.

The use of numerical methods in palaeontology is well established and has been used to address a wide range of palaeontological problems (Harper 1999; Hammer &

Harper 2006). Ideally, a systematic sampling programme should be undertaken to provide data for rigorous quantitative analysis of palaeoecological data (Etter 1999). Although the BGS collections were not assembled as part of such a sampling exercise, a set of standard numerical exploratory techniques (see Hammer & Harper 2006, p. 6) was applied to the macrofaunas in these collections from the Hurlet and Index limestones in western Scotland (Figs 1, 2) to determine whether recurrent faunal assemblages could be recognised and reasonable interpretations made in terms of palaeoenvironments and lithofacies. The results of the analysis compare favourably with the published qualitative results of Wilson (1967; 1989) whose understanding was founded on a wealth of experience ‘based on innumerable observations made over forty years’ (Wilson 1989, p. 111).

The Hurlet and Index limestones: a review of the collected palaeontological materials

The Hurlet (Brigantian) and Index (Pendleian) limestones mark the bases of the Lower and Upper Limestone formations respectively (Fig. 2), and have been correlated over most of central Scotland (see Wilson 1967; 1989; Browne *et al*. 1999). Both limestones occur at the southern margin of the Ayrshire Coalfield (Fig. 1), which is a region of current geological resurvey and 3D computer modelling by the British Geological Survey. The analysis of the macrofaunal assemblages forms part of that work.

The fossils are mainly held in the Biostratigraphy collections in the British Geological Survey office in Edinburgh (see Dean 2002). They were collected from 67 localities (14 for the Hurlet Limestone and 53 for the Index Limestone) over a period of approximately 136 years. The sample localities include both borehole and surface exposures. The material from each locality was subdivided by hand specimen lithology into mudstone/claystone (undifferentiated), calcareous mudstone, sandstone, siltstone, calcareous siltstone, limestone, argillaceous limestone, and dolostone. This resulted in 20 macrofaunal samples for the Hurlet Limestone and 94 samples for the Index Limestone. Fossil content was tabulated on a spreadsheet arranged by genera and species within major groups, each determination being made to the highest level of confidence at the localities sampled. For lists of localities, taxa and sample lithologies used in this study see Supplementary material.

The data were compiled over time at the most detailed taxonomic level possible for each locality and so range from records of named species to indeterminate material ascribed only to a phylum. The limitations of the data owing to the gradual acquisition of samples to the collection rather than palaeoecologically focused bulk sampling (e.g. Etter 1999) include:

- Samples differ in dimensions from pieces of core of various diameters to hand specimens of various sizes. It cannot be discounted that at least some of the differences among samples reflect differences in sample dimension, which at present are not quantified but are very variable.
- Specimens from the same locality were not necessarily obtained from the same bed.
- Taxonomic identifications in the database were undertaken by many palaeontologists working on Carboniferous fossils since 1870. Hence they are polythetic and in most instances are not underpinned by systematic monographic studies or ecophenotypic analysis of the material. For older determinations the

taxonomy may in some cases need updating.

- The collections lack any taphonomic assessment such as the degree to which the fossils were autochthonous or allochthonous.
- Crucially, only presence/absence (binary) data are available and this provides a major limitation on the range of numerical methods that can be applied.

Consolidation and restriction of the data sets

To overcome limitations of sample size and limited taxonomic overlap between samples in the exploratory analyses, which aim to identify similarities between groups of samples, successive iterations of the analyses were undertaken on increasingly consolidated or restricted versions of the original data.

The species- and genus-level data were consolidated by removing records of indeterminate brachiopods, bivalves and gastropods where named taxa of these groups were recorded from the same sample. If a species was unequivocally identified at any locality in the species-level data set, that name was also applied to all other ‘aff.’, ‘cf.’ and ‘?’ determinations applied to that binomen. Next, all taxa restricted to a single locality were excluded so that the analyses of these ‘unique taxa excluded’ data were based solely on shared occurrences thus reducing considerably the amount of ‘noise’ in the data. In addition, the genus-level ‘consolidated’ data were further restricted to higher level taxa (essentially a mixture of phyla and classes), with the number of genera present in each group recorded rather than simple presence or absence. This provides a measure of diversity within the higher taxa and is amenable to ordination using PCA as well as cluster analysis based on quantitative data.

Numerical methodology

The consolidated data in binary (presence/absence) format was analysed using the statistical package *PAST* (*PAlaeontological STatistics*) (Hammer *et al*. 2001), which is available on the Internet as freeware, is periodically updated and refined, and is fully supported by an extensive manual.

Four data sets, comprising the Hurlet Limestone species and genera, and Index Limestone species and genera, were transferred into PAST and analysed as described below. Seriation, cluster analysis and to some extent non-metric multidimensional scaling (NMDS) proved suitable techniques for use on the binary data, whilst cluster analysis and PCA were appropriate for the diversity data within high level clades.

Seriation reorganises the original binary data matrix to group shared presences of taxa along a diagonal. Unconstrained optimization enables the ordering of both the taxa and localities to achieve a best fit and the ordering of the localities reflects their position along a palaeoecological, palaeobiogeographical and/or temporal gradient. The fewer the influencing factors (such as water depth, substrate characteristics, salinity and oxygenation), the better the clustering along the diagonal and therefore the higher the fitness criterion computed for the seriation. These fitness criteria are therefore much higher for the consolidated data than for the preliminary analyses, which included taxa unique to any one locality. For example, the species-level seriated matrices gave fitness a criterion of 0.721 for the consolidated data compared with 0.397 for the raw, unconsolidated, data for the Hurlet Limestone palaeontological data set and 0.288 cf. 0.139 for the equivalent Index limestone data set. When the samples were subdivided by lithology, consolidation generated fitness criteria on the seriations of 0.635 cf. 0.285 and 0.17 cf. 0.11 for the Hurlet and Index limestones respectively. Constraining the seriations, by fixing the ordering of samples of a particular lithology, forces the grouping of other lithologies. For example, constraining the limestone subset in the species-level seriated matrix for the Hurlet Limestone using the consolidated data set with unique taxa excluded reduced the fitness criterion from 0.635 to 0.403. However, this constrained analysis resulted in the grouping of other lithologies, suggesting ranges of lithofacies tolerance for individual species.

Q-mode analysis was used in the cluster analyses to distinguish groups of samples with similar faunas. Three similarity indices, Dice, Simpson and Raup-Crick, were employed and the clusters joined using the un-weighted pair group average (UPGMA) algorithm. The Dice coefficient was used in the NMDS where persistent patterns in the resultant two dimensional plots of ranked (rather than absolute) difference between samples were taken to reflect genuine structure within the data.

PCA is a widely used eigenvector technique, which operates on a correlation or variance-covariance matrix (Davis 1986) to identify as much of the variation in a set of data and to seek structure within the samples (see Hammer & Harper 2006). The first principal component is always orientated in the direction of maximum variation in the sample; the second and subsequent components are perpendicular to the first, explaining decreasing amounts of variation. As is common in such analyses, the first two or three eigenvectors in the present study contained most of the sample variation.

In the first instance, the 'palaeontological' data fields for both the Hurlet and Index limestones were analysed prior to possible links to lithology being explored. The latter involved subdividing the faunal lists from many of the localities in terms of the lithology of the rocks in which each fossil is contained. This increases the information attached to each faunal occurrence but decreases many of the sample sizes and diversities.

Results

Palaeontological data alone

Most of the Hurlet Limestone samples are lithologically homogenous and 33% of species and 36% of genera in the original palaeontological data set occur at multiple localities. By consolidating the data, the percentage of shared genera increases to 46%. Excluding taxa restricted to single localities produced minor changes in the order of the localities and higher fitness criteria in the seriated data (e.g. Fig. 3) together with more consistency of clustering among different similarity coefficients used in the cluster analyses (Fig. 4). The last of these is encouraging given the different emphases that these coefficients have in terms of co-occurrences, relative sample size or the mathematical processes involved (e.g. see Hammer & Harper 2006, pp. 212–213). Three groups of localities were consistently identified in the various seriations and are also recognised by NMDS. Group 1, which also emerges consistently in the cluster analyses (Fig. 4) comprises Carskeoch (locality 12), Daldilling (26), Nethershield (55), River Ayr (Windy Burn) (65) and Windy Burn (67); Group 2 comprises Cairnshalloch Limeworks (9), Captain's Glen (11), Dailly Station (24), Heronspark Burn (36), Meikleholm Burn (52) and Quarrelhill Burn (57);

Group 3 comprises Auchmillanhill Bore (1), Captain’s Bridge (10) and River Ayr (Upper Heilar) (64).

These three groups of localities were discriminated purely on the basis of their faunal association but there are some broad links between these faunal associations and lithofacies:

(i) Group 1 is a fauna characteristic of clearer water conditions with a preferrence for a firm substrate. It is linked to a wide range of lithologies, particularly limestone;

(ii) Group 2 is a fauna characteristic of clear water conditions with a preferrence for a soft substrate. It is linked to an association of limestone-dominated lithofacies;

(iii) Group 3 is a low diversity fauna with a preference for muddier water conditions and a soft substrate. It is linked to a siliciclastic lithofacies.

These results closely mimic the seminal semi-quantitative analysis published by Wilson (1989), who presented, in generalised diagrammatic form (Wilson 1989, fig. 9), the occurrence of the most commonly found marine fossils of the Dinantian of central Scotland in relation to the lithology of the host rocks. He related the fossils, at group and genus-level, to the lithology they were found in (mudstones and limestones with increasing or decreasing calcareous and siliciclastic content). From this he deduced their living environments on the continental shelf, which ranged from a nearshore zone with muddy water, to offshore or nearshore zones with clearer water. The parallels between the quantitatively determined groupings of faunas recognised in the BGS collections in the present study and those recognised by

Wilson with his wealth of field experience demonstrate that geologically significant patterns can be recognised in the historical palaeontological data sets not originally collected for this purpose.

Restricting the genus-level consolidated data to higher taxonomic groups and recording the number of genera present in each group, provided a measure of diversity within the higher taxa (Fig. 5) that was amenable to cluster analysis and PCA (Fig. 6). The grouping of localities evident in the species- and genus-level analyses were not generally preserved in the cluster analyses of the quantitative data, but two large groups of localities were distinguished. These also form non-overlapping portions of the plot of the second and third components of the PCA. Some differentiation of the samples is provided by the third component. These include gastropods at localities 10, 12 and 52 with loadings around zero; anthozoans and bryozoans at localities 65 and 67 with low positive loadings; and nautiloids and others at localities 9, 24 and 57 with higher positive loadings.

In contrast, however, the picture was far from clear for the lithologically more heterogeneous Index Limestone, a thicker depositional unit with a much larger number of samples. No clear palaeoecological patterns emerged from the five associations discriminated in the solely palaeontological data by cluster analysis.

Inclusion of lithological data

Subdividing the samples on the basis of the lithology containing the fossils provides an explicit link between faunal associations and a potentially very important facet of the palaeoenvironment.

Hurlet Limestone

The unconstrained seriations of consolidated data at both species- and genus-level for all taxa from the Hurlet Limestone are very similar and have fairly low fitness criteria of 0.33 and 0.35 respectively. Excluding taxa restricted to any one locality produces a large increase in the fitness criterion to 0.635 and 0.617 respectively (Figs 7, 8). Apart from the distinction of siltstone samples in the genus-level seriation there is no grouping of samples by lithology. Constrained seriation, based on the order of the limestone samples that emerged from an unconstrained analysis of the limestone samples alone produces a grouping of the other lithologies (Figs 9, 10) albeit with lower fitness criteria than the equivalent unconstrained seriations. The seriations show that tolerance ranges of some taxa within the carbonate environments extend into other lithofacies in a systematic way across environmental gradients.

Cluster analyses of species- and genus-level data sets (all taxa and unique taxa excluded) do not reveal consistent patterns. However, recurring groupings of samples emerge from cluster analysis of the numbers of genera within higher taxa. Application of both the Dice and Raup-Crick coefficients to this ‘higher taxa’ data set show three major clusters (Ht 1–Ht 3), five sub-clusters (Ht 1.1–Ht 3.1), and five close pairings (Ht 1.1.1–Ht 3.1.2) (Fig. 11). The three major clusters can also be recognised on the unconstrained seriation of the whole data set and even more closely in the subset of limestone samples. Again this suggests changing co-occurrences of taxa across an environmental gradient.

The first three components of the PCA represent 93% of the variation within the 'higher taxa' data set from the Hurlet Limestone, with 81 % represented by Principal Component 1. The main variables along these three principal components are, in turn: (1) brachiopods; (2) bivalves; and (3) crinoids and bryozoans (with algae, foraminifera and crustaceans). The major clusters identified in the cluster analysis (Ht 1, Ht 2 and Ht 3, Fig. 13) can also be recognised on the PCA plots (Fig. 12); their distributions reflecting differences in trophic structure of the faunal associations (and therefore differences in environment). Both the cluster analysis and PCA of the diversity data reveal three major clusters that account for all but 2 of the samples. These groups cut across lithofacies but reflect differences in taxonomic composition and trophic structure.

- Ht 1 includes seven samples. The lithofacies represented are limestone (with dolostone) (57%) and argillaceous limestone, mudstone/claystone (undifferentiated)/calcareous mudstone, and siltstone (about 14% each). The fauna includes brachiopods (59% of all genera recorded within the cluster) with 1–9 genera present in each sample, bivalves (21%) with 0–3 genera, and crinoid columnals (13%) with 0–1 genera.
- Ht 2 includes seven samples. The lithofacies represented are argillaceous limestone (43%), limestone (29%) and calcareous sandstone and siltstone (14% each). The fauna includes mainly brachiopods (93%) with 1–4 genera, and gastropods (7%) with 0–1 genera.
- Ht 3 includes five samples. The lithofacies represented are limestone (80%) and mudstone/claystone (undifferentiated) (20%). The fauna includes mainly brachiopods (63%) with 1–8 genera, crinoids (19%) with one genus, and bryozoa (11%) with 0–2 genera.

Index Limestone

The fitness criteria for the unconstrained seriations of the species- (0.06) and genus- (0.11) level data sets for all taxa and even for the data with the unique taxa excluded are very low (species 0.17 and genera 0.20), and none show grouping of samples from similar lithologies. Constraining the genus-level seriation by the ordering determined for the limestone samples alone results in most of the other lithologies grouping together, but the fitness criterion is extremely low (0.10) and there is no clear relationship between lithofacies and faunas. However, the broad grouping of the lithologies suggests that some taxa were distributed along environmental gradients within the carbonate depositional setting and extended outside it into other sedimentary environments in a non-random way.

The results of cluster analyses of all the species- and genus-level data sets do not show any consistent groupings. However, cluster analysis of the higher taxa 'diversity' data set using both the Dice and Raup-Crick coefficients shows eight nested clusters (Ix 1.1–Ix 2.6) of three or more samples (Fig. 13) within two major clusters (Ix 1 and Ix 2), broadly reflecting differences in lithology. This suggests there is a crude link between lithology and the diversity and distribution of genera among the higher taxa.

Most of the variation in the 'higher taxa' data set for the Index Limestone is expressed by components 1 and 2 of the PCA which together comprise almost 89% of the variance in the data; the third component accounts for 4%. The main loadings on these components are, sequentially: (1) brachiopods and bivalves (strong positive loading); (2) brachiopods (strong negative loading); and (3) gastropods. The major and nested clusters discerned in the cluster analysis can also be distinguished to some extent on the PCA plots (Fig. 14). In general, the most calcareous mudstone faunas in the Index Limestone are mainly included in major cluster Ix 1 and are of low diversity with brachiopods the dominant or sole component and molluscs generally absent. Sandstones and especially siltstones are mainly included major cluster Ix 2 and have moderate to high diversities of brachiopods and bivalves with gastropods present in some cases.

Palaeoecological and palaeoenvironmental interpretation of the structure identified in the collections

Hurlet Limestone

The lithofacies and environmental gradients of taxa selected from the genus-level constrained seriation of the unique taxa excluded data set are shown in Figure 15. These taxa are included in the three faunal groups previously identified, and their palaeoecology accords with the interpretations of Wilson (1989).

The dominant taxa, general trophic structure and palaeoenvironment occupied by the groups of samples identified by cluster analysis of the higher taxa data set (Fig. 11) and to a large extent recognisable in the PCA plots (Fig. 12) can be summarised as follows:

- Ht 1 contains brachiopods and bivalves and, in most samples, crinoid columnals. The epifaunal brachiopods will have colonised a range of substrates depending upon whether they were pedunculate or free lying, but the bivalves are considered to represent infauna with a preference for more muddy substrates. The lithologies of the samples suggest that this major cluster represents a great range of environments, but mainly clear water in the off- or nearshore zones.

- Ht 2 is dominated by brachiopods indicating a range of substrates depending upon whether they were semi-infaunal, pedunculate or free lying. Gastropods also occur, which may have preferred to graze or plough carbonate mud.
- Ht 3 is of epifaunal forms, mainly brachiopods and crinoids most of which will have flourished on firmer substrates.

Index Limestone

Seriation of all the consolidated genus-level data with the samples constrained to the order obtained by seriating the limestone samples alone suggests that the faunal gradients within the carbonate depositional environments can be extended into increasingly coarse siliciclastic sediments. Figures 16 and 17 show this for taxa that have, respectively, an extensive and a limited range within the carbonate environment.

The major clusters and their sub-clusters identified in the cluster analysis for the higher taxa data set are at least partially recognised on the ordination of samples on the PCA and show links between faunal associations and lithologies that reflect the exploitation of subtly different environments. A detailed analysis of the composition and trophic structure of the clusters will form part of a separate study; suffice it to note here that:

Ix 1 is dominated by brachiopods and includes mainly calcareous lithofacies. The limestone lithologies indicate clearer water, the offshore or nearshore zones, firmer substrates, and dominant epifaunal forms. The slightly calcareous mudstone and mudstone/claystone (undifferentiated) lithologies provide evidence of the intermediate to muddy nearshore zones, the latter especially with less firm substrates dominated by infaunal forms. The siltstone lithology of a single sample provides almost insignificant evidence of a zone considered to represent river sediment influx.

Ix 2 is dominated by brachiopods and various molluscs. It includes mainly calcareous lithofacies, but with a significant proportion of siliciclastic sedimentary rocks. The limestone, and slightly calcareous mudstone and mudstone/claystone (undifferentiated) lithologies are indicative of the same palaeoenvironments and faunal associations as for Ix 1. The siltstone and sandstone lithologies show a siliciclastic environment in what is considered to represent a zone of river sediment influx.

Conclusions

- Exploratory numerical techniques can be successfully applied to historical palaeontological collections (not originally intended to investigate palaeoecology) to distinguish palaeoecologically meaningful faunal associations and their palaeoenvironmental setting.
- Records of sample locality and lithology (‘environmental data’) and fossil content (described by major fossil groups, genera and species) can be used; the limitations of sample size, taxonomic overlap and solely binary (presence or absence) data being minimised by excluding all ‘one off’ occurrences of fossil taxa and analysing increasingly consolidated or restricted versions of the original information.
- Seriation, cluster analysis and NMDS are suitable techniques for use on

binary data, whilst the distribution of genera within higher taxonomic groups can be used as a proxy for abundance data to distinguish meaningful faunal associations using cluster analysis and PCA.

- Seriation can be used to indicate the lithological and environmental gradients of some taxa. Cluster analysis can reveal groups of samples, linking lithology and the diversity and distribution of taxa. PCA can explain the distribution of the clusters in terms of differences in taxonomic composition, trophic structure, lithology and environment.
- Quantitative analysis of the historical BGS collections from the Hurlet and Index limestones confirms the relationship between lithofacies and palaeoenvironment inferred by Wilson (1989) and enables the recognition of more subtle patterns not identifiable by qualitative means.
- The success of this study unlocks the potential for palaeoecological interpretation by multivariate numerical analysis of historical collections not originally intended to investigate palaeoecology. An example of such a collection is that of the BGS, where a vast resource, originally collected for biostratigraphy, now awaits renaissance in palaeoecology.

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Figure captions:

FIG. 1. The geology of the Ayrshire Coalfield Basin including the crop of the Hurlet and Index limestones and the sample localities. Graticule is British National Grid. For full details of the sample localities see Supplementary material.

FIG. 2. Stratigraphical framework for the Ayrshire Coalfield Basin including up-to-date lithostratigraphical nomenclature. Based on Browne *et al.* (1999, table 1); Holliday & Molyneux (2006, fig. 1).

FIG. 3. Hurlet Limestone. Species-level seriated matrix for the unique taxa excluded data set. Fitness criterion = 0.721. For locality details see Supplementary material.

FIG. 4. Hurlet Limestone. Species-level cluster analyses for the unique taxa excluded data set, using the Dice, Simpson, and Raup-Crick coefficients.

FIG. 5. Hurlet Limestone. Data matrix for the diversity analysis showing the higher taxa, localities and numbers of genera within each taxon at those localities. For locality details see Supplementary material.

FIG. 6. Hurlet Limestone. Plot of first and second components in the PCA of the number of genera in the higher taxa. The numbered localities are listed in Figure 4. Contours delimit the number of higher taxa in each group.

FIG. 7. Hurlet Limestone. Species-level seriated matrix for the unique taxa excluded

data set. Fitness criterion = 0.635. Lithological abbreviations: CMdst = calcareous mudstone; CSlst = calcareous siltstone; Dst = dolostone; Lst = limestone; Mdst = mudstone/claystone (undifferentiated); MLst = argillaceous limestone; Slst = siltstone; Sst = sandstone. For sample and taxonomic details see Supplementary material.

FIG. 8. Hurlet Limestone. Genus-level unconstrained seriated matrix for the unique taxa excluded data set. Fitness criterion = 0.617. For lithological abbreviations see Figure 7. For sample and taxonomic details see Supplementary material.

FIG. 9. Hurlet Limestone. Species-level seriation to observe lithological groupings of taxa using all samples constrained, for the unique taxa excluded data set. Fitness criterion = 0.403. For lithological abbreviations see Figure 7. For sample and taxonomic details see Supplementary material.

FIG. 10. Hurlet Limestone. Genus-level seriation to observe lithological groupings of taxa using all samples constrained, for the unique taxa excluded data set. Fitness criterion = 0.426. For lithological abbreviations see Figure 7. For sample and taxonomic details see Supplementary material.

FIG. 11. Hurlet Limestone. Cluster analysis for the higher taxa data set used in the diversity analysis, using the Raup-Crick coefficient. For sample details see Supplementary material. Ht 1–3: major clusters of samples; Ht 1.1–3.1: nested clusters of samples; Ht 1.1.1–3.1.2: close pairings of localities.

FIG. 12. Hurlet Limestone. Plot of: (a) the first and second principal components, and (b) the second and third principal components in the PCA of the numbers of genera present in higher taxa showing the fields occupied by samples belonging to the three major clusters (Ht 1–3) identified in Figure 11. For sample details see Supplementary material.

FIG. 13. Index Limestone. Cluster analysis for the higher taxa data set used in the diversity analysis, using the Raup-Crick coefficient. For sample details see Supplementary material. Ix 1–2: major clusters of samples; Ix 1.1–2.6: nested clusters of samples. Note that Ix 1.1 and Ix 1.2 together contain most of the argillaceous limestone samples, with Ix 1.2 containing most of the calcareous mudstone samples. Ix 2.1–2.6 contain most of the siltstone and sandstone samples.

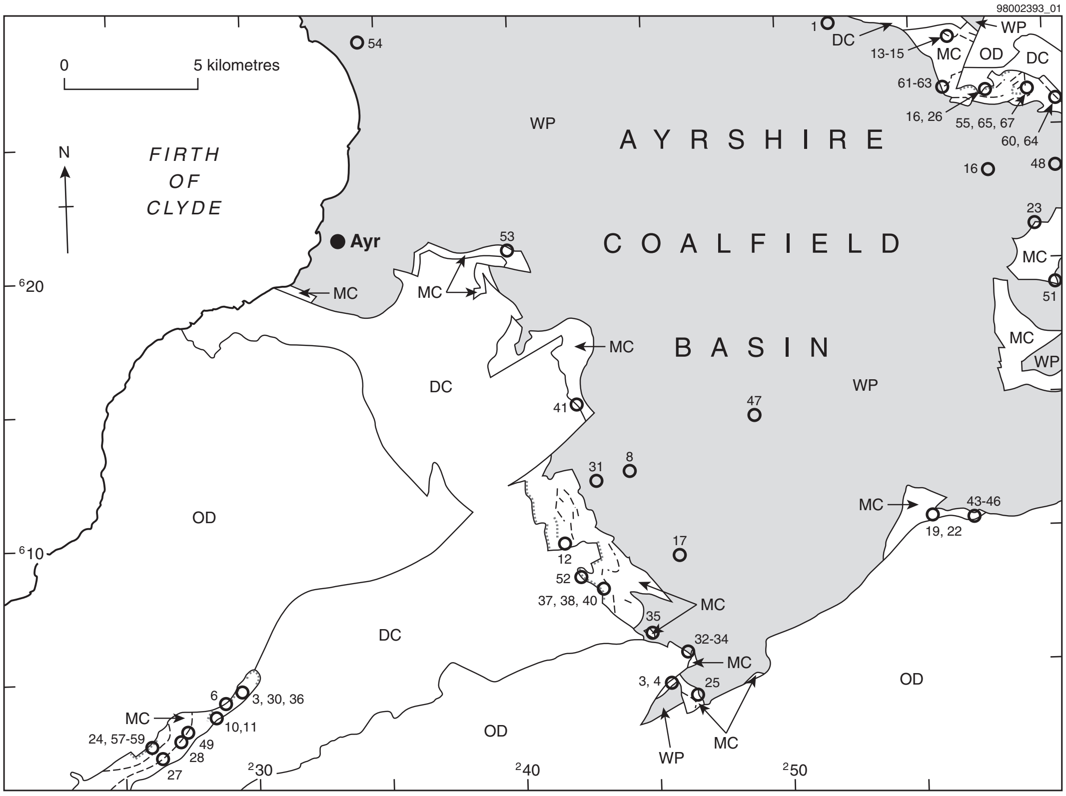
FIG. 14. Index Limestone. Plot of: (a) the first and second principal components, and (b) the second and third principal components in the PCA of the numbers of genera present in higher taxa showing the fields occupied by the two major clusters (Ix 1–2) identified in Figure 13. For sample details see Supplementary material.

FIG. 15. Hurlet Limestone. Ranges of lithofacies and environments of the taxa selected from the genus-level seriation using all samples constrained, for the unique taxa excluded data set. The dotted lines indicate interpolated presence.

FIG. 16. Index Limestone. Faunal gradients of taxa that have the most extensive range within the carbonate depositional environment and extend increasingly into the siliciclastic depositional environment. Based on a seriation of all the consolidated

genus-level data, the samples being constrained to the order obtained by seriating the limestone samples alone. The dotted lines indicate interpolated presence.

FIG. 17. Index Limestone. Faunal gradients of taxa that have a limited range within the carbonate depositional environment and extend furthest into the coarse siliciclastic depositional environment. Based on the seriation of all the consolidated genus-level data, the samples being constrained to the order obtained by seriating the limestone samples alone. The dotted lines indicate interpolated presence.



WP	Westphalian-Permian rocks	DC	Devono-Carboniferous (including Courceyan to Brigantian) rocks	··········	Crop of the Hurlet Limestone
MC	Middle Carboniferous (including Brigantian to Arnsbergian) rocks	OD	Ordovician-Devonian rocks	– – – – –	Crop of the Index Limestone
				o	Sampling locality

Standard Divisions			Subsystem (obsolete)	Regional Divisions			Lithostratigraphical Units	
Sub-system	**Series**	**Stage**		**Series**		**Stage**	**Formations**	**Groups**
Pennsylvanian	Middle (*pars*)	Moscovian (*pars*)	Silesian	Westphalian	C	Bolsovian	Scottish Upper Coal Measures	Scottish Coal Measures Group
	Lower	Bashkirian			B	Duckmantian	Scottish Middle Coal Measures	
					A	Langsettian	Scottish Lower Coal Measures	
				Namurian		Chokierian-Yeadonian	Passage Formation	Clackmannan Group
Mississippian	Upper	Serpuk-hovian				Arnsbergian	Upper Limestone Formation	
								Index Limestone
						Pendleian	Limestone Coal Formation	
	Middle	Viséan	Dinantian	Viséan		Brigantian	Lower Limestone Formation	
								Hurlet Limestone
							Lawmuir Formation	Strathclyde Group
						Asbian	Kirkwood Formation	
						Arundian-Holkerian	Clyde Plateau Volcanic Formation	
	Lower	Tournaisian		Tournaisian		Chadian	Clyde Sandstone Formation	Inverclyde Group
						Courceyan	Ballagan Formation	
							Kinnesswood Formation	

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Locality \ Taxon	*Buxtonia* sp.	?*Pugilis* sp.	trepostomatous bryozoa	*Avonia youngiana*	orthotetoid	gigantoproductoid	athyrid	spiriferid	crinoid columnals	*Pleuropugnoides* sp.	productoid	*Spirifer bisulcatus?*
65	■	■	■	■	■	■	■		■			
26	■			■	■				■			
67		■	■	■	■	■		■	■			
55				■				■				
12					■	■		■	■			
52							■		■			
11							■		■	■		
24								■	■		■	
57									■	■	■	
9									■		■	
36									■			■
10											■	
1											■	■
64												■

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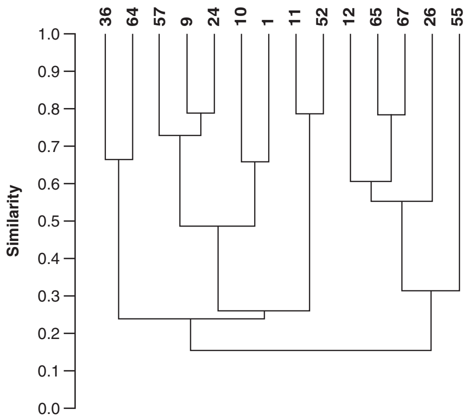
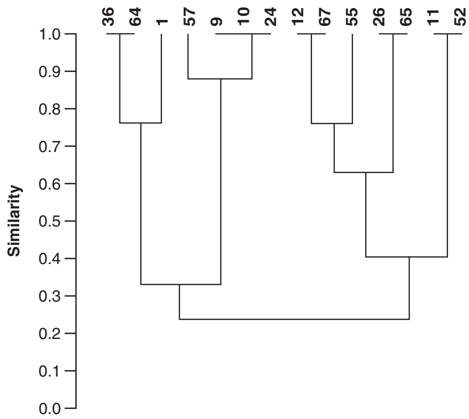
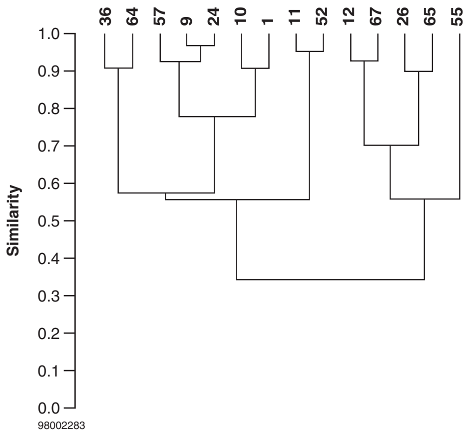
Dice



Simpson



Raup-Crick



Localities

1 Auchmillanhill Bore
9 Cairnshalloch Limeworks
10 Captain's Bridge
11 Captain's Glen
12 Carskeoch
24 Dailly Station
26 Daldilling
36 Heronspark Burn
52 Meikleholm Burn
55 Nethershield
57 Quarrelhill Burn
64 River Ayr (Upper Heilar)
65 River Ayr (Windy Burn)
67 Windy Burn

Locality / Taxon	ALGAE	FORAMINIFERIDA	ANTHOZOA	BYROZOA	BRACHIOPODA	GASTROPODA	BIVALVIA	NAUTILOIDEA	CRUSTACEA	CRINOIDEA
1	0	0	0	0	2	0	1	0	0	0
9	1	1	0	0	1	0	1	1	1	1
10	0	0	0	0	1	1	1	0	0	0
11	0	0	0	0	2	0	0	0	0	1
12	0	0	0	0	3	1	1	0	0	1
24	0	0	0	0	3	0	0	1	0	1
26	0	0	0	0	3	0	3	0	0	1
36	0	0	0	0	1	0	0	0	0	1
52	0	0	0	0	5	1	1	0	0	1
55	0	0	0	0	4	0	0	0	0	0
57	0	0	0	0	2	0	1	1	0	1
64	0	0	0	0	1	0	1	0	0	0
65	0	0	1	1	8	0	0	0	0	1
67	0	0	0	2	5	0	0	0	0	1

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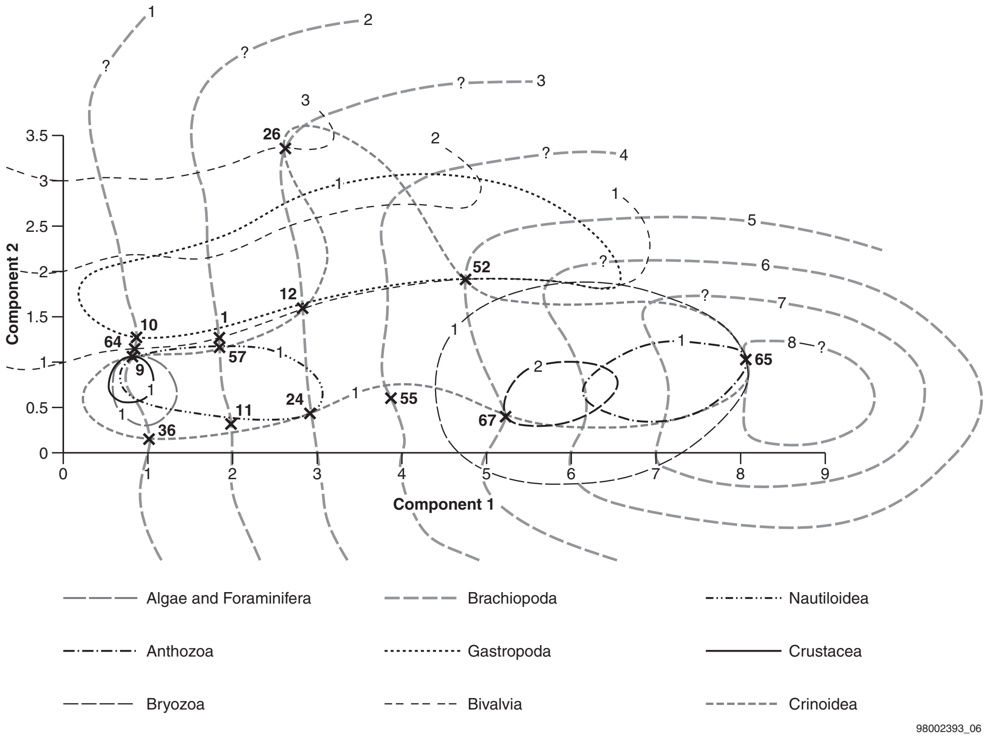

Component 2
Component 1
3.5
3
2.5
2
1.5
1
0.5
0
0
1
2
3
4
5
6
7
8
9
26
10
64
9
1
57
12
52
24
11
36
55
67
65
Algae and Foraminifera
Brachiopoda
Nautiloidea
Anthozoa
Gastropoda
Crustacea
Bryozoa
Bivalvia
Crinoidea
98002393_06

Sample / Taxon	gigantoproductoid	?*Pugilis* sp.	trepostomatous bryozoa	*Avonia* sp.	*Buxtonia* sp.	orthotetoid	athyrid	rhynchonellid	*Avonia youngiana*	crinoid columnals	*Camarotoechia* sp.	orthocone nautiloid	*Composita* sp.	spiriferid	productoid
67aMLst	■														
12bLst	■					■									
65aLst	■	■	■	■	■	■	■	■		■					
67bLst		■	■			■			■	■					
26aMLst				■	■					■					
52aLst							■	■		■					
65cCSlst								■	■						
11aLst							■			■	■				
36aLst										■					
12aMdst										■					
1aMdst/CMdst						■		■		■		■	■	■	■
55aLst									■					■	
57aLst										■	■	■	■		■
9aLst										■					■
65bMLst													■		
24aLst										■				■	■
67cSlst														■	
64aSlst														■	
10bMLst															■
10aDst															■

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Sample \ Taxon	gigantoproductoid	*Buxtonia*	trepostomatous bryozoa	*?Pugilis*	*Avonia*	orthotetoid	athyrid	rhynchonellid	crinoid columnals	*Camarotoechia*	orthocone nautiloid	*Composita*	spiriferid	productoid
67aMLst	■													
12bLst	■					■								
65aLst	■	■	■	■	■	■	■	■	■					
26aMLst		■			■				■					
67bLst			■	■	■	■			■					
55aLst	■				■								■	
65cCSlst					■			■						
52aLst							■	■	■					
11aLst							■		■	■				
12aMdst									■					
36aLst									■					
1aMdst/CMdst						■		■	■		■	■	■	■
57aLst									■	■	■	■		■
9aLst									■					■
65bMLst												■		
24aLst									■				■	■
64aSlst													■	
67cSlst													■	
10aDst														■
10bMLst														■

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