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Towards a statistically valid method of textural sea floor characterization of benthic habitats

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Abstract

Multibeam bathymetric sonar technology and benthic habitat research require the systematic characterization of the seafloor, necessitating reliable and accurate sea floor descriptors in combination with a robust means to statistically assess descriptor associations. Historically, geoscientific sea floor characterisation involves identifying the spatial extent and relationship of geological units, broadly following litho– or chronostratigraphic criteria, but these conventions may not be meaningful biologically because they incorporate temporal elements that stem from a geochronological qualifier. Textural properties of geological facies are typically given in terms of distribution-dependent statistics, which have been shown to be inappropriate with multimodal marine sediments, such as on glaciated shelves. As habitat classification is aimed at boundary definition, the boundaries between groups in such cases could be arbitrary, or based on very subtle differences, or noise (e.g., sampling bias). This study uses an independent statistical approach pioneered by Calinski and Harabasz (C–H) which offers significant advantages in determining the appropriate number of groups that might exist in any sample population. Used in conjunction with a multivariate extension to information-entropy, grain size populations can be clustered into statistically validated groups. This study utilizes a 30-yr legacy of 4-class grain size data collected from the Scotian Shelf, Canadian Atlantic continental margin, we show that a traditional stratigraphic approach does not provide clear discrimination between basic textural types, and hence, basic benthic habitats. Considerable improvements in textural zonation are obtained using a combination of information entropy-clustering and C–H technique. Two high resolution, 32-class particle-size data sets yield a solution where no obvious textural groups exist, contrary to published field-based studies. Comparison of sediment grab samples to bottom photographs from other shelf sites show that photos capture (sample) a wider range of textural variability, particularly the coarsest-gravel component that is sometimes absent from grabs, and therefore, classification from photos creates more groups. This study emphasizes that data resolution and sea-floor sampling strategies should be intimately linked, and to fully unravel high-resolution textural data might require in excess of a four order of magnitude increase in the number of bottom sediment samples. Therefore, data should be collected at the highest practical resolution but be reduced to a resolution meaningful for statistical analysis, in accordance with the total sample population.

Keywords: Grain size; Benthic habitat; Sea floor; Statistics; Cluster analysis; Scotian Shelf

1. Introduction

The advent of modern multibeam technology and the thematic development of benthic habitat analysis have spawned renewed interest in the systematic char-

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acterization of the seafloor (e.g., Greene et al., 1995; Todd et al., 1999; Kostylev et al., 2001). Increased interest in seafloor benthos and bio-physical interactions has focused interdisciplinary studies on new morphological detail and sediment textural attributes (e.g., Kostylev et al., 2003). Such an approach necessitates the application of reliable and accurate sea floor descriptors in combination with a robust means to statistically assess descriptor associations. Historically, geoscientific sea floor characterization was primarily concerned with the identification, spatial extent, and geometrical relationship of geological units, broadly following litho- and chronostratigraphic conventions. However, for the purposes of delineating different benthic habitats, more emphasis is placed on sediment texture as an indicator sea floor type that now necessitates robust and statistically meaningful classification techniques.

Sediment grain size is a key descriptor of seabed texture but commonly only one granulometric parameter, such as mean grain size or sorting, are being applied in correlations to benthos and acoustic backscatter response (e.g., Todd et al., 1999; Kostylev et al., 2003). However, on many continental shelves, and in particular those with a glacial signature, sediments have bimodal or polymodal size distributions, placing significant limitations on these traditional distribution-dependent statistics. Most of the grain-size moment measures and granulometric parameters were formulated using sieve technology. Hence, as emphasised by Forrest and Clark (1989), the need arises for a statistically robust technique to characterize a complex size distribution as readily as a simple one, a procedure that accounts for the total information contained within the distribution curve, and a technique that deals efficiently with the limitations in the input data.

Procedures derived from information theory and using an entropy statistic to define clusters of similar samples can offer significant advantages with grain size data (e.g., Sharp, 1973; Pelletier, 1974; Forrest and Clark, 1989; Woolfe and Michibayashi, 1995). In particular, a multivariate extension to such an approach overcomes the problem of pre-selecting the optimal number of class intervals common to all samples in the data set (see Full et al., 1983). A multivariate technique will group samples in terms of the totality of their distributions, irrespective of the optimal number of intervals for particular samples. In addition, the technique allows the flexibility to group other semi-quantitative data (provided they are normalized).

Benthic habitat analysis emphasizes animal-soft sediment relationships, and some of the complexities of these associations and problems that arise in their interpretation are comprehensively summarized in Snelgrove and Butman (1994). Classifying seafloor sediments following geological conventions may not be meaningful biologically because they often incorporate formation age, chronological relationship to glacially-lowered sea level, or sediment genesis. Geological nomenclature and classification was established following lithostratigraphic or chronostratigraphic criteria that may not be closely related to grain size and/or benthos.

A complex suite of glaciogenic materials, variably reworked by marine processes occurs on the Scotian Shelf along the eastern coast of Nova Scotia, Canada (e.g., King, 1970; Fader et al., 1977; Fader, 2004). A historical emphasis on geological mapping has yielded a 30-yr legacy of grain size data, derived from sediment grab samples, dredges, and cores. In addition, recent multibeam surveys have produced bathymetric and backscatter data across significant areas of the shelf providing an invaluable proxy for texture. As a supplement to characterising surficial geological units on the Scotian Shelf, Kostylev et al. (2001) attempted to examine the relationship of sediment to acoustic backscatter and benthic habitat, using a semi-quantitative categorization of sediment texture. The advantages of adopting such an approach were inconclusive for several reasons, namely: (1) similar backscatter patterns used as a proxy for grain size could be produced by different seabed morphologies and mean grain sizes (2) complex mixtures of grain types and size modes can lead to variability in the size-frequency distribution that are unreliably represented by mean grain size, particularly in glacially-influenced multimodal sediments; (3) many species are characteristically associated with a given sedimentary habitat, although their distributions are rarely confined to that environment (Snelgrove and Butman, 1994; Newell et al., 1998). For example, as a generalization, suspension feeders favour coarser substrate whereas deposit feeders prefer finer substrate, but the boundaries between these assemblages will often be gradational and complex. Hence, while the relationship between sediment grain size and biota appears intuitively-evident, traditional granulometric properties (e.g., mean grain size) alone do not appear to be a determinant of species distribution or community composition. These studies emphasize the need for a robust and statistically meaningful technique to describe soft-substrate texture if relationships to benthos are to be better understood and quantitatively assessed.

The present study attempts to explore a more meaningful measure of the seabed physical texture that will potentially improve seabed characterization and correlation to benthic assemblages. This also facilitates the creation of statistically valid geospatial maps, where appropriate. Habitat classification is aimed at boundary definition, but the classification process is problematic because most statistical clustering techniques will, by their very nature, form clusters, which may or may not represent a meaningful difference between groups. Boundaries generated between clusters could be based on minor differences, be arbitrary or, in the worse case, reflect noise in the data (e.g., sampling bias, analysis techniques, measurement error, etc.). Here, we propose a revised method that addresses the need for a repeatable and objective method of classification, combined with a statistically valid and independent means of assessing the number of meaningful groups. Therefore, the statistical validity of the clustering outcomes can be tested at each step of the classification scheme. In addition, we examine the effects of data resolution resulting from archiving 32-class high-resolution data as reduced 4-class summaries.

2. Classification methodology

Samples were sorted into self-similar groups by entropy analysis, an approach pioneered by Shannon (1963), and more recently adapted as a QBASIC computational program by Woolfe and Michibayashi (1995). This computer-based approach has its roots as a FORTRAN-executed, multivariate extension to information theory by Semple et al. (1972), which was later modified by Johnston and Semple (1983). Unlike other grouping techniques, entropy analysis minimizes the amount of within-group variance by testing for all possible groupings of samples.

For the univariate case, the inequality of a distribution, $I(Y)$ can be obtained using Eq. (1)

$$I(Y) = \sum_{i=1}^{N} Y_i \log_q N_{Yi} \tag{1}$$

where, Y_i is the proportion of grains for sample Y in a size category i, or the probability of any event occurring in interval i; N is the number of size intervals ($i=1, 2, \ldots, N$); and, q is any base logarithm (base 2 as adopted by Forrest and Clark, 1989; Woolfe and Michibayashi, 1995).

For the multivariate case described by Semple et al. (1972), with N size intervals and K samples, the total-inequality statistic is given by Eq. (2)

$$I(Y) = \sum_{j=1}^{J} Y_j \sum_{i=1}^{N} Y_i \log_2 N Y_i \tag{2}$$

where: Y_j is the frequency value (of grains in this case) in size intervals (column) j; J is the number of intervals; N is the number of samples; Y_i is the frequency value (of grains) in size interval (column) j that are in sample (row) i, such that $Y_i = Y_{ij} / Y_j$; where Y_{ij} is the proportion of the total population (of all K samples) in row i, column j. Then

$$\sum_{j=1}^{J} Y_j = 1.0 \text{ and } \sum_{i=1}^{K} Y_i = 1.0 \tag{3}$$

$I(Y)$ is thus the inequality in the distribution of size intervals across all samples, weighted by the frequency of samples in each size category. Given the number of groups (r), derivation of the weighted inter-row inequality value allows the calculation of between-group inequality $I_B(Y)$ from

$$I_B(Y) = \sum_{j=1}^{J} X_j \sum_{r=1}^{M} Y_{jr} \log_2 \frac{Y_{jr}}{\frac{N_r}{N}} \tag{4}$$

where M is the maximum number of groups considered. The procedure optimizes the classification of the N samples into r classes (groupings of samples) through maximization of between-class and minimization of within-class entropy. Following Forrest and Clark (1989), a statistically optimum grouping is attained when the growth rate of the between-group entropy significantly decreases with the addition of yet further groups. The adaptation of Woolfe et al. (1998a,b, 2000) of the multivariate extension of Semple et al. (1972) introduces an addition term, the R_s statistic, which is the percentage of the dataset "explained", which is defined numerically as:

$$R_s = \frac{\text{between group inequality}}{\text{total inequality}} \times 100. \tag{5}$$

Graphically this approximates the inflection point in a plot of the number of groups versus the percentage explained (e.g., Woolfe et al., 1998a,b, 2000). General agreement with field observations of sediment textural facies has also been used as an additional semi-quantitative measure of the appropriate number of meaningful textural subdivisions (e.g., Woolfe et al., 1998a; Orpin et al., 1999, 2004). However, as noted by Full et al. (1983), with complex frequency distributions, as is the case with multimodal sediments, a complementary method for determining the optimal number of groups is required. To that end, in the present study we adopt a method using a C–H criterion derived by Calinski and Harabasz (1974), which is the pseudo F-statistic of multivariate analysis of variance and canonical analysis. A study of a wide range of clustering criteria by Milligan and Cooper (1985) showed that the C–H pseudo F-statistic provided a consistent and reliable indication of the appropriate number of groups. Moreover, in seafloor characterisation applications, Legendre et al. (2002) have demonstrated the usefulness of the C–H statistic in acoustic sediment classification.

The C–H pseudo F-statistic is defined by the ratio of the mean square for the given grouping divided by the mean square of the residuals (Eq. (6))

$$\mathrm{C{-}H} = \frac{\left[\dfrac{R^2}{(K-1)}\right]}{\left[\dfrac{(1-R^2)}{(n-K)}\right]} \tag{6}$$

where n is the number of samples, K is the number of groups into which samples were clustered, and

$$R^2 = \frac{(\mathrm{SST}-\mathrm{SSE})}{\mathrm{SST}} \tag{7}$$

where, SST is the total sum of the squared distances to the overall centroid (similar to the total inequality or the between groups sum of the squares), and SSE is the sum of the squared distances of the objects to the groups own centroids i.e., within group sum of the squares. It follows then, that the grouping in which the C–H statistic is at a maximum, is the optimal grouping solution in terms of a least-squares solution (similar to a pseudo F-test), and has no significance value associated with the C–H statistic. Visual examination of a plot of C–H statistic vs. the number of classes provides an optimal definition at the highest point on the C–H curve. In general, an overall higher C–H value indicates a greater degree of order in the data array, with random data having a C–H statistic around an order of magnitude less than non-random or ordered data. In addition, for the present study, a permutation test was designed for evaluating the likelihood of the C–H statistic being greater than that expected from a random allocation of the existing data into grain size classes.

3. Regional setting

The Scotian Shelf of the Canadian east coast margin covers approximately 160,000 km^3, broadens in width from 125 km in the southwest to 230 km at its northernmost end, and the shelf break occurs between 140–180 m water depth (Fig. 1). Like many formerly glaciated continental shelves, the Scotian Shelf is characterized by a series of large, shallow banks separated by troughs and basins, and can be delineated into three physiographic zones (after King and MacLean, 1976): an inner zone characterized by rough topography; a central zone of isolated banks with irregularly-shaped intervening basins and valleys; and, an outer zone consisting of a series of wide, flat and shallow banks (Fig. 1). Mid-shelf basins reach 290 m water depth, and some are interpreted to lie in the path of former major ice streams, and their basin-shape the result of glacial erosion (King et al., 1974). Outer shelf banks shoal to 27 m, and in the case of Sable Island are subaerially exposed. The Quaternary lithostratigraphy for the Scotian Shelf was originally defined by King (1970), primarily on the acoustic echo characteristics and shallow bottom samples, and was later applied and adapted to the Gulf of Maine (Fader et al., 1977) and the Grand Banks (Fader et al., 1984). While these lithostratigraphic units have significant regional extent, variations have been observed in the nearshore zone and on the outer parts of Sable Island Bank and Banquereau (summarized in Piper et al., 1990). Surfacial sediments are comprised of five basic lithostratigraphic units, namely: LaHave Clay, Sable Island Sand and Gravel, Sambro Sand, Emerald Silt, and Scotian Shelf Drift (after King and Fader, 1986; King, 1970). Sediment facies maps have been published for the Scotian Shelf which follow lithostratigraphic conventions (e.g., Fader, 2004) (Fig. 1a). Of particular note in the present study, is the application of textural characteristics to delineate these facies.

4. Data sources

In the present study we examine a number of particle-size datasets from different environments, sub-sampled using different methodologies including van Veen, IKU, and Shipek grab samplers, and box, gravity, and piston corers. Grain sizes were measured using traditional sieve, settling, and sedigraph techniques. These comprise a verified archive of 1917 samples collected from the northeastern sector of the Scotian Shelf on the eastern Canadian continental margin over the past 3 decades (Fig. 1b). Typically data are archived at Wentworth arithmetic size intervals of gravel (<4 mm), sand, silt, and clay. By way of comparison, two datasets based on high resolution 32-class output from a laser-particle sizer from tropical Australia (after Orpin et al., 1999, 2004) are also discussed. In addition, a dataset of 246 bottom grain size descriptions (8 particle size sub-classes) estimated from seabed photographs (after Rumbolt and Kostylev, 2004; Fig. 1c), and 465 quantitative estimates of benthic biomasses (5 taxonomic classes) from grab and dredge samples (after Stewart et al., 2001; Fig. 1d), collected from the Scotian Shelf are

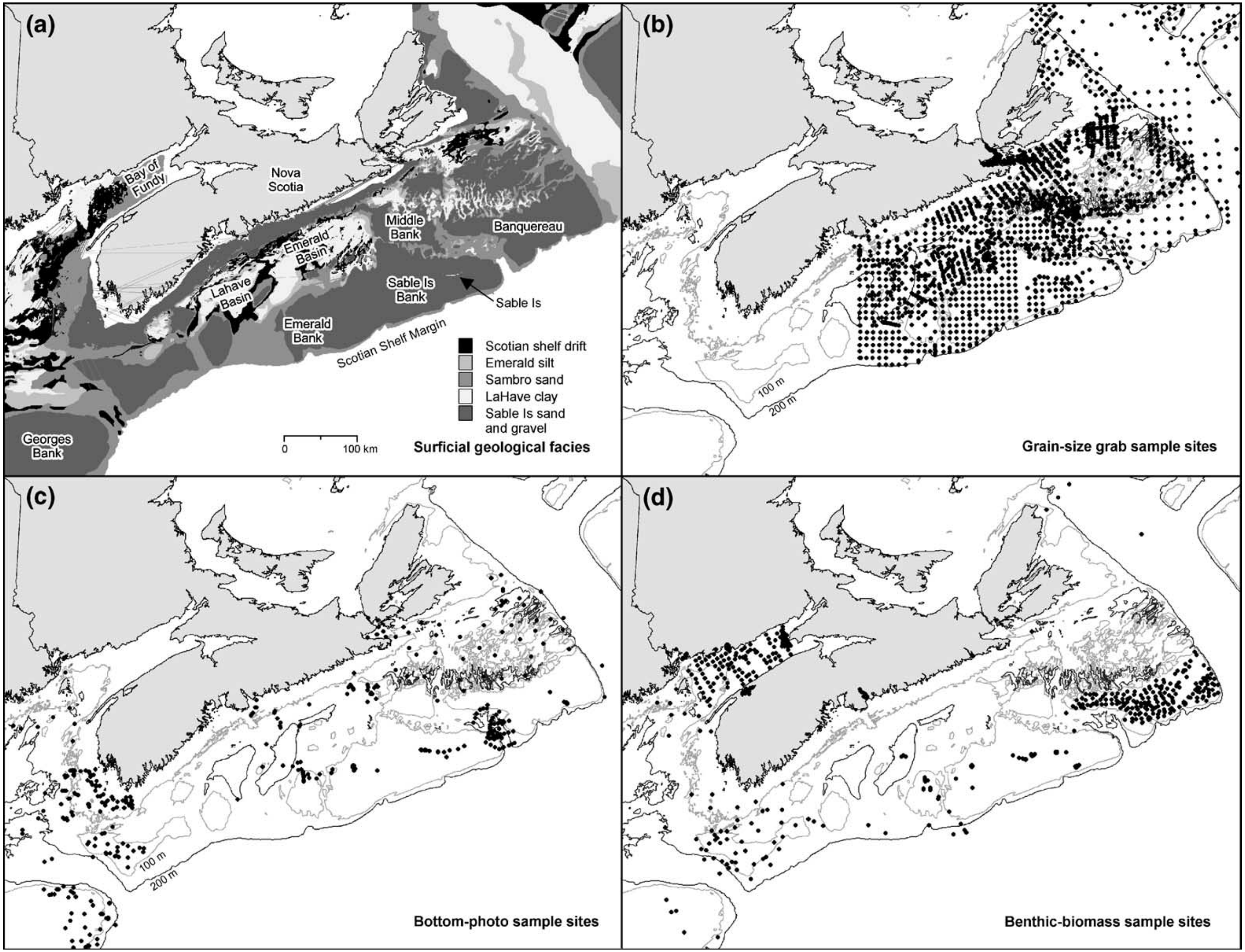

Fig. 1. Locality map of the Scotian Shelf of the Canadian east coast margin. The surficial geological sediment facies are indicated (after Fader, 2004) along with the localities of the 1917 grain-size grab samples, 246 bottom photographs, and 465 benthic biomass sample sites.

included to show the validity of the classification technique with other data types. Samples for grain size, bottom photograph, and biomass were collected from different sample sites (Fig. 1), at different scales, and from a range of geological and biological studies. While not ideal for comparative purposes, this type of historical data archive is institutionally very common. Rather than reducing the impact of our approach, it places even greater emphasis on statistically valid methods of characterization so that spatially-gridded data (coverages) can be quantitatively assessed in a modern GIS environment.

To make a quantitative assessment of possible textural characterization bias resulting from different grain size resolutions, 32-class size data from the Great Barrier Reef (after Orpin et al., 2004) were reduced to 4 broad classes (clay, silt, sand, course sand) that covered the same size range as the original (4–2000 μm). Artificial (synthetic) datasets were also created to assess the ability of the grouping methodology to identify a priori known groups. Similarly, random datasets were employed to test the ability of the characterization technique to disregard random noise and continuous variability, yielding a result that favoured the selection of one group.

5. Results

Entropy analysis in conjunction with C–H statistics allows the determination of the optimal classification of the samples into self-similar groups. Where real and well-defined groups exist in the dataset the C–H statistics gradually increase until reaching a maximum value. In addition, statistical tests were computed to assess the probabilities of the C–H statistic being higher than that

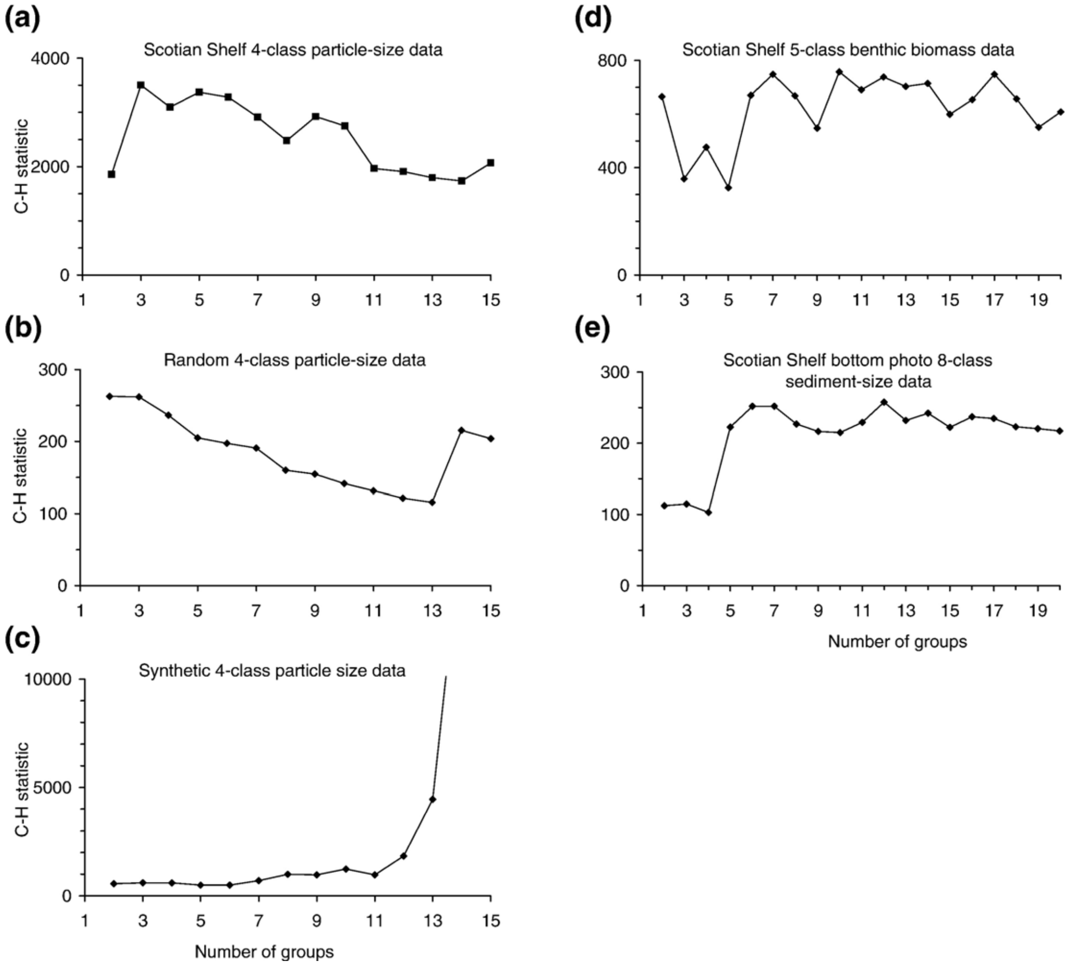

Fig. 2. Curves of the Calinski–Harabasz (C–H) pseudo F-statistic for the following data: (a) the 4-class Scotian Shelf size data; (b) randomly generated 4-class size data; (c) pre-defined 15-group, 4-class size data; (d) 5-megafaunal group, 5-class benthic biomass data; (e) 7-class sediment cover estimated from bottom photographs. The grouping optimum solution is attained when the C–H statistic is a maximum.

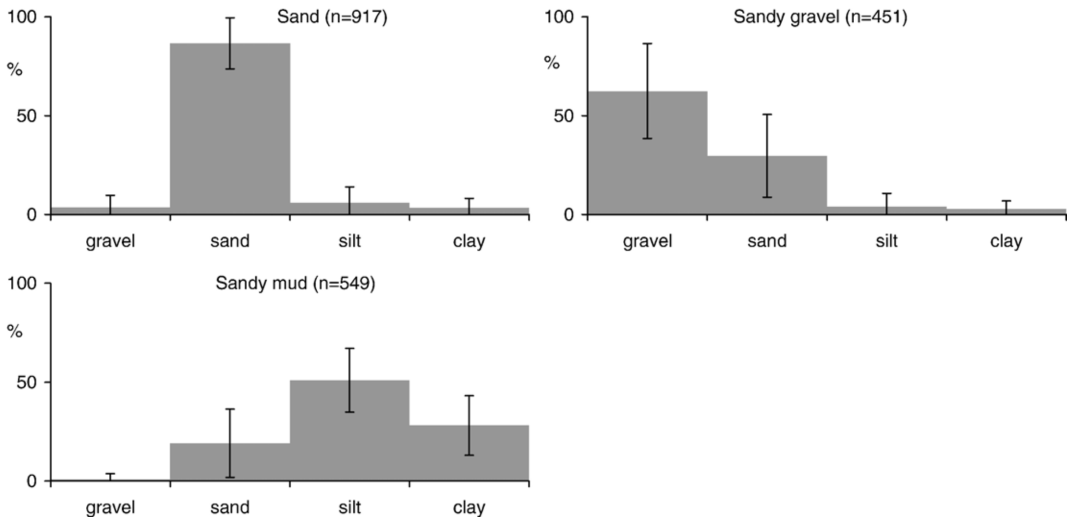

Fig. 3. Entropy-derived textural facies for the Scotian Shelf. Three basic textural facies can be recognized: sand, sandy gravel, and sandy mud. Within-class variability is indicated by the error-bars of one standard deviation from the mean frequency percentage value, and "*n*" denotes the population of samples within each group.

of random data. For the Scotian Shelf, utilizing four-class data (clay, silt, sand, and gravel), the best grouping solution yields three groups, and further division shows a trend of decreasing C–H statistic (Fig. 2a) with a local maximum at nine groups. Comparison to an equivalent number of randomly-generated 4-class data yields a curve that shows that the C–H statistics attains the maximum value at the first subdivision of the data (2 groups) and then gradually declines (Fig. 2b). The absolute values of the C–H statistics are approximately

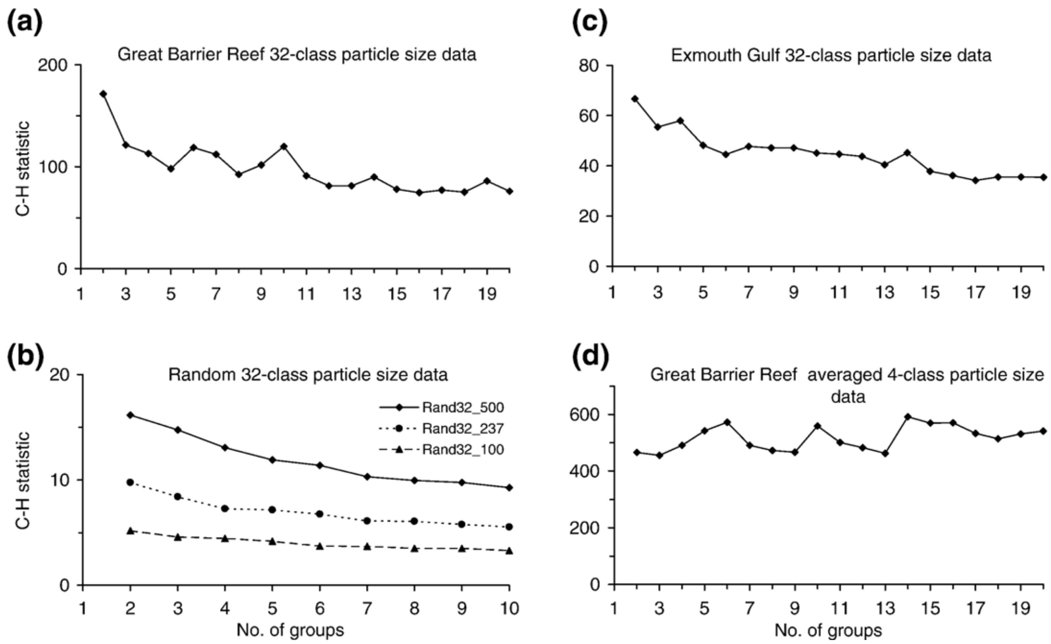

Fig. 4. Curves of the Calinski–Harabasz (C–H) pseudo *F*-statistic for the following data: (a) 32-class laser-derived particle size data from the Great Barrier Reef, Australia (data from Orpin et al., 2004); (b) randomly-generated 32-class size data. For Great Barrier Reef data, the shape of the C–H curve shows the maximum C–H statistic occurs with a 2-group solution, and a progressive decrease upon successive subdivision into more groups. However, small local peaks occur also at 6, 10, and 14 groups in both the 32-class and the corresponding reduced 4-class datasets; (c) 32-class laser-derived particle size data from Exmouth Gulf, northern Western Australia (data from Orpin et al., 1999); and, (d) reduced 4-class, mean data from the Great Barrier Reef.

an order of magnitude less than those calculated from the Scotian Shelf data. The probabilities of the C–H statistic being higher than that of randomly permutated data are zero, confirming that even the C–H maximum in this classification is not indicative of optimal grouping of the samples. Rather, there are no real groupings in the dataset to be distinguished. Note the sharp increase that occurs at 14 groups (Fig. 2b), which could represent a weak harmonic in the random data set. Similarly, a synthetic 4-class dataset (with 15 predefined groups) shows an incremental increase in C–H statistic from 1 to 14 groups, but reaches infinity at 15 groups when the perfect solution is found and the within-group variability is zero (Fig. 2c). By way of comparison, the absolute value of the C–H statistic is an order of magnitude larger than that of random data. The benthic biomass of five groups of megafauna and sediment cover data estimated from bottom photographs yield a maximum C–H statistic of 7 and 6 groups, respectively (Fig. 2d, e), and show more variability than the simple 3-textural groups for the Scotian Shelf.

The entropy-derived textural facies for the Scotian Shelf shows that the groups form the basic classes of sand, sandy gravel, and sandy mud (Fig. 3). Within-group variability is high for sandy mud and sandy gravel facies, as indicated by the larger within-class standard deviation.

Examination of the Calisksi–Harabasz (C–H) pseudo F-statistic shows that the probability of the C–H statistic being higher than that of “random data” was 1 for 237 Great Barrier Reef samples and 153 samples from Exmouth Gulf. For Great Barrier Reef data (Fig 3a), the shape of the C–H curve shows the maximum C–H statistic occurs with a 2-group solution, and a progressive decrease upon successive subdivision into more groups but small, local peaks occur at 6, 10, and

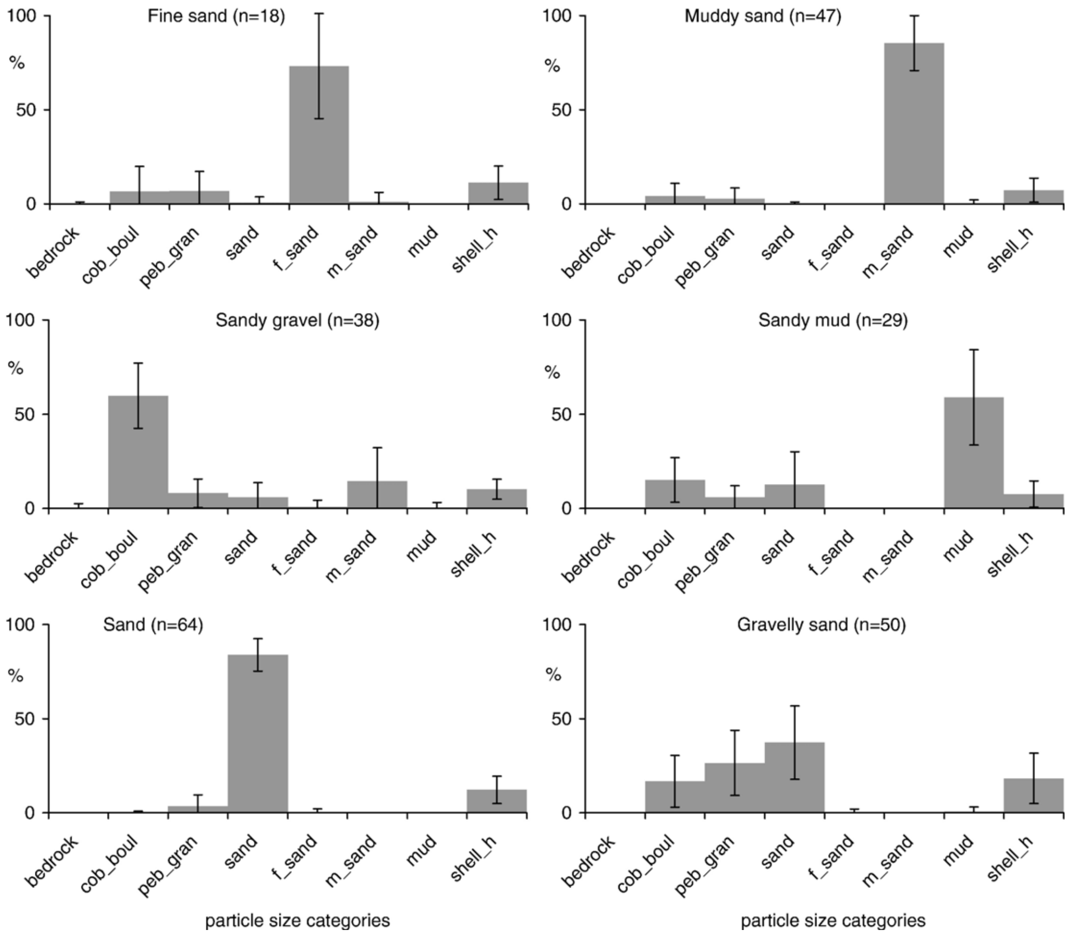

Fig. 5. Entropy-derived sediment facies from sediment cover estimated from 8-textural class bottom photographs. Six basic textural classes can be recognized: fine sand, muddy sand, sandy mud, sand, gravelly sand, and sandy gravel. Within-class variability is indicated by the error-bars of one standard deviation from the mean frequency percentage value, and “n” denotes the population of samples within each group.

14 groups (Fig. 4a). Comparison to randomly generated data (Fig. 4b) with an equivalent number of samples to the Great Barrier Reef (237) shows that the field data C–H statistics were significantly higher than random (up to an order of magnitude), indicating that although all 20 classifications were signifi cant, the 2-group solution was optimal. Experimentation with the number of samples employed in the C–H analysis indicates that an increase in the number of random samples to 500 (approximately double) produces a small increase in the amplitude of the C–H statistic (Fig. 4b). Similarly, a decrease to 100 random samples (approximately half) results in a small reduction in the amplitude of the C–H statistic (Fig. 4b). By comparison, the C–H statistics for Exmouth Gulf size data (Fig. 4c) are lower in amplitude, but the progressive decrease in the C–H statistic is similar to the Great Barrier Reef. Reducing the Great Barrier Reef data from 32 to 4 broad classes (clay, silt,

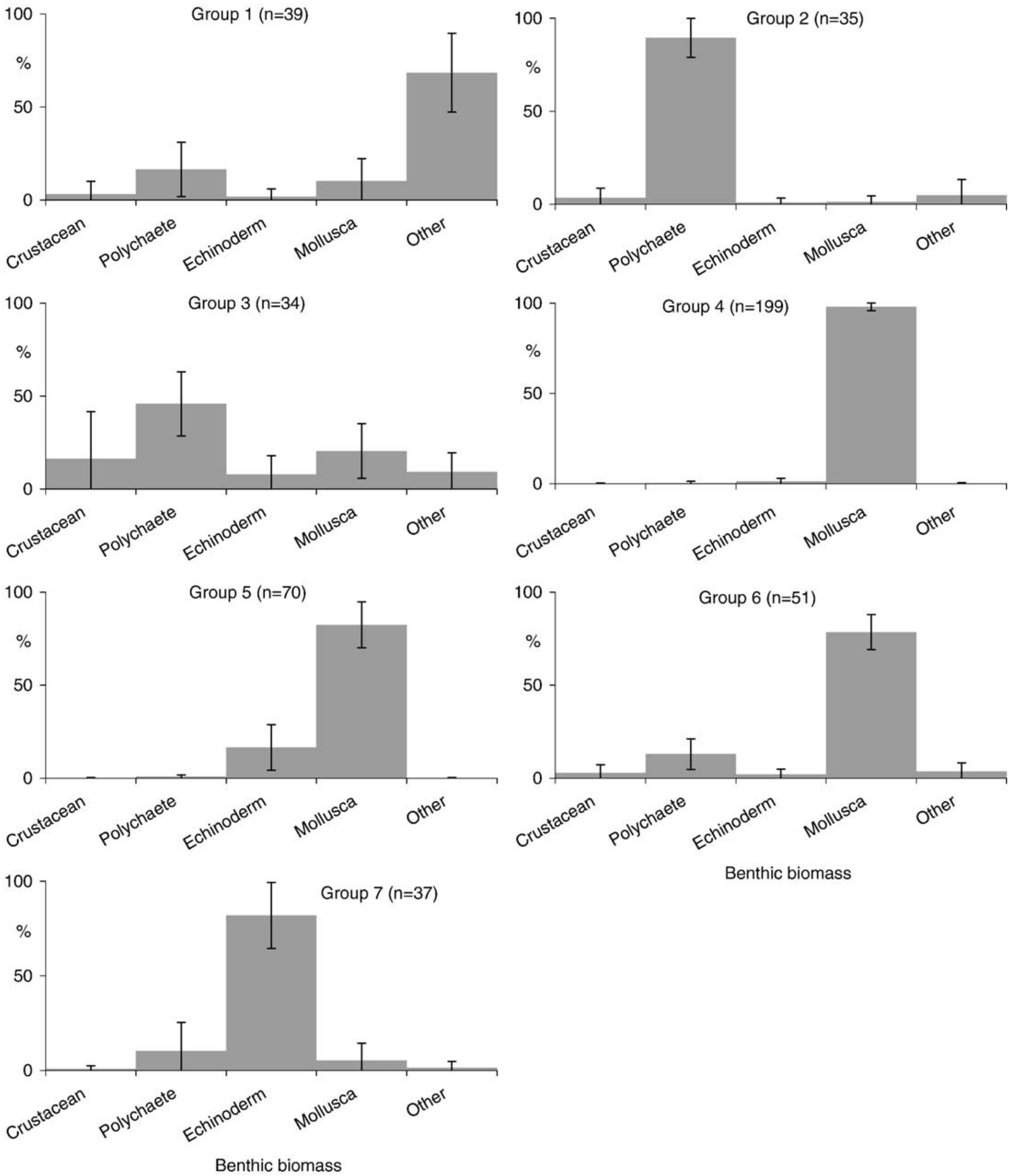

Fig. 6. Entropy-derived benthic biomass types derived from five groups of megafauna. Seven basic textural types can be recognized. Within-class variability is indicated by the error-bars of one standard deviation from the mean frequency percentage value, and "*n*" denotes the population of samples within each group.

sand, very coarse sand) shows that an optimal C–H statistic is attained at 6 groups (Fig. 4d) with local peaks at 6, 10 and 14 groups. In addition, there is a five-times increase in the amplitude of the C–H statistic. This contrasts to the minimal group solution observed in the original 32-class data (Fig. 4a). This analysis suggests that the amplitude of the C–H statistic has a positive relationship to the number of samples and a negative relationship with the number of classes within each sample. In essence, data order increases upon the addition of more samples and a reduction in resolution (number degrees of freedom).

The entropy-derived groups for sediment cover obtained from bottom photograph observations of the Scotian Shelf show 6 broad textural facies (Fig. 5). Within-group variability is most apparent in two textural facies that contain a gravel component, and least variable (best sorted) in sand-dominated facies (Fig. 5). The 7 entropy-derived groups of benthic biomass from the Scotian Shelf suggest taxonomic variability (within-

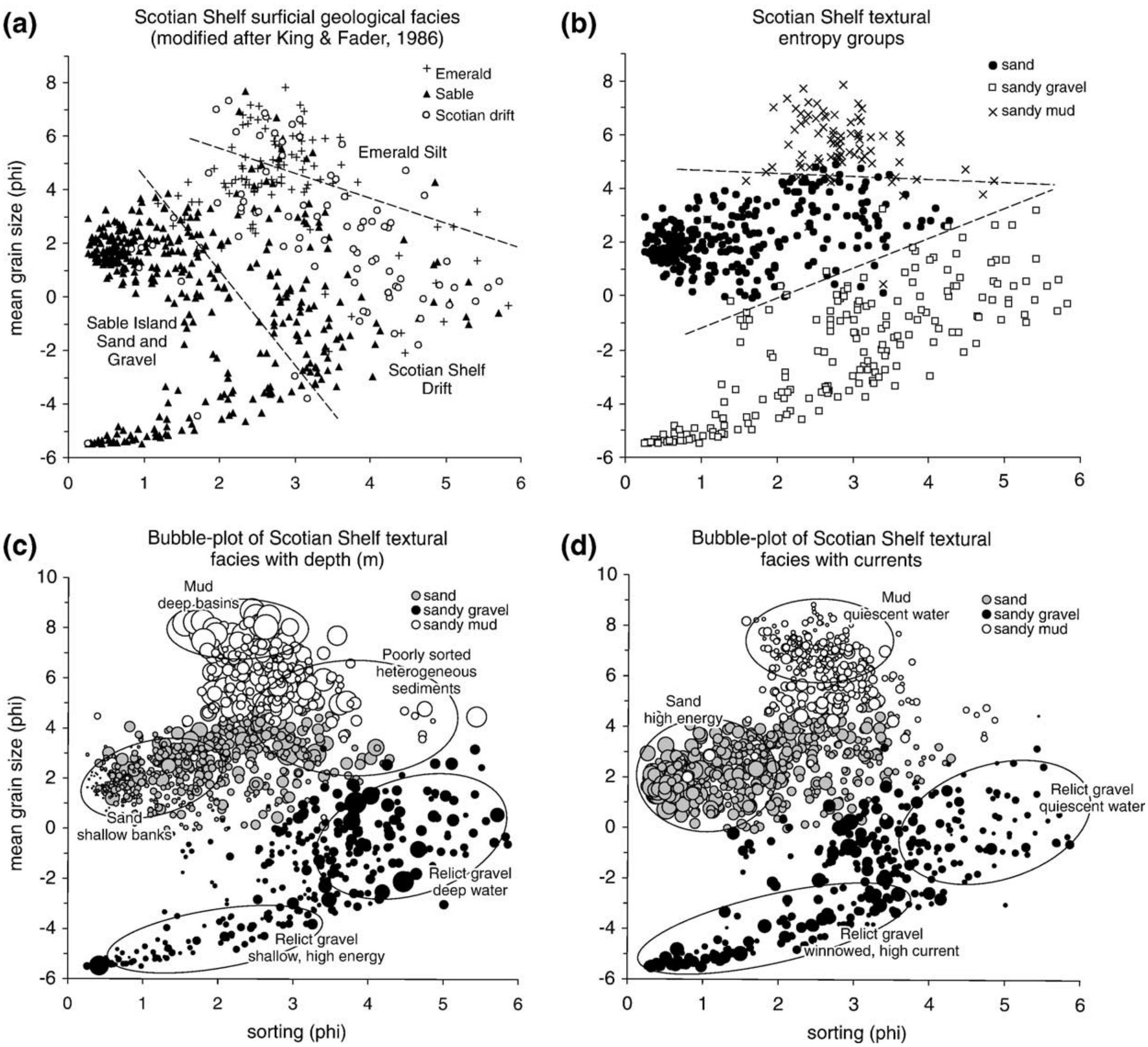

Fig. 7. Textural discrimination plots of the same Scotian Shelf bottom samples: (a) grouped according to geological units with inferred facies boundaries (modified after King and Fader, 1986); (b) grouped according to entropy-derived facies groups, with inferred textural boundaries; (c) bubble-plot of entropy-derived facies with the addition of water depth (a large bubble diameter represents deep water, maximum of 500 m); and, (d) bubble-plot of entropy-derived facies with the addition of current strength (a large bubble diameter represents a fast current, maximum of 24 cm/s). The entropy-derived textural facies have considerably less overlap than using a chronostratigraphic classification. Scotian Shelf current data were derived from a regional oceanographic model and were kindly provided by C. Hannah (Department of Fisheries and Oceans, pers. commun. 2004).

group variability) is lowest in molluscan- or polychaete-dominated habitats (groups 2, 4 and 6, Fig. 6).

King and Fader (1986) applied a textural discrimination plot to identify geological facies described from core and grab samples from the Scotian Shelf. In general, Scotian Shelf drift was noted as being very poorly sorted, Sable Island Sand and Gravel were generally better sorted (King and Fader, 1986), and finer-grained Emerald Silt formed a discrete textural field. An adaptation of this discrimination plot, using the same facies boundaries and ascribed chronostratigraphic sedimentary units shows that considerable textural variability exists across the Scotian Shelf upon the addition of further grab sample sites (Fig. 7a). This arises because the graph now incorporates many grab sample stations that have undergone significant post-depositional reworking at the seabed by waves and currents. Many of these samples were "filtered out" in the original plot presented by King and Fader (1986) (G. Fader, pers. comm., 2004). This underscores the limitations of the stratigraphic approach in characterizing the upper few centimeters of substrate. Entropy classification of the same samples shows three distinct textural facies with considerably less overlap than using chronostratigraphic units (Fig. 7b). Sandy gravels show the greatest within-group variation in both sorting and mean grain size, and sandy mud the least. Two boundaries that demarcate the textural facies can be inferred, which, in contrast to King and Fader (1986), form predominantly along trends in mean-grain size (Fig. 7b). The addition of a third dimension to this graphical approach in the form of a bubble plot summarises additional environmental information. The inclusion of water depth (Fig. 7c) and inferred currents (Fig. 7d) reinforces basic environmental trends, whereby: well-sorted, shallow-water gravels occur in areas of high energy, whereas poorly sorted gravels are typical of deep quiescent water; well sorted sands occur on high energy, current swept banks; muds are typical of deep quiescent basins; and, a large group of poorly-sorted heterogeneous medium sands and fine sediments occur at intermediate depths. While this grouping presents an improved tool for relating benthic habitat it must be viewed in the context of a strong imprint of early post-glacial reworking processes, that continue locally today.

6. Discussion

Key to the application of physical information for the construction of benthic habitat maps is the quantity and quality of data required to produce a meaningful result. Textural characterization of the seafloor is no different, but in addition suffers from a bias that stems from its traditional measurement and application in sedimentological studies. Even today, many studies have used only one distribution-dependent measure to classify the texture of the sea bed (e.g., Kostylev et al., 2001; Porter-Smith et al., 2004). In this study we support the use of the entire size envelope in addition to traditional measures, and have attempted to classify the sea bed into texturally self-similar groups. However, an overriding question remains: how much textural information is required to obtain a meaningful result i.e., can a reliable result be obtained from traditional 4-class (clay, silt, sand, gravel) rather than modern, multi-binned, laser-derived data? In many cases a 4-class format will exist in long-established archives, determined using a range of traditional methods including sieves, pipette, and X-ray sensing (i.e., Sedigraph) technologies. Collectively, these data still form a valuable data resource for regional benthic habitat characterisation.

Using information entropy yields three textural classes for the 4-class Scotian Shelf sediments. In this example, the collaborative implementation of the C–H criteria provides a mathematically independent measure of the likely number of "real" discrete groups, which can easily be assessed from the plot of C–H versus the number of groups (Fig. 2a). Similarly, bottom photograph and benthic biomass 8- and 5-class data, respectively, yield C–H curves that are more complex with several local highs (inflections). This could be a result of the greater resolution offered by the data. However, larger data matrices of high-resolution 32-class grain size data from the Great Barrier Reef and Exmouth Gulf yield unexpected results (Fig. 4a, c). Here, in both cases the "optimum" solution is obtained at only 2 groups, the least complex grouping beyond a continuous single distribution. At first glance this appears counterintuitive as presumably these large data arrays contain considerably more information. Moreover, published sedimentological studies using these same data have identified several discrete textural facies that appear to be mappable on the shelf at a regional scale (e.g., Orpin and Woolfe, 1999; Orpin et al., 1999, 2004). The reduced 4-class form of the Great Barrier Reef data yields a curve that indicates 6 groups are statistically favoured (Fig. 4d), which is also a local peak in the grouping solutions for the larger 32-class data array. Similarly, there are corresponding peaks at 10 and 14 groups. Hence, the reduction to 4-class data appears to have the most profound effect on the shape of the C–H curve for 1–4 group solutions and on the amplitude of C–H values.

One possible explanation for this behaviour is that the increased resolution leads to the inherent increase of the within-group variability, which in turn may lead to a potentially misleading C–H statistic. As an experimental outcome, this contrasts with the earlier applications of C–H techniques, where perhaps due to computational limitations, lower-resolution data arrays with fewer number of groups were explored. By the very nature of the C–H calculation, the amplitude of the C–H statistic increases linearly with increasing number of samples. However, to successfully account for the within-group variability in high-resolution data statistically necessitates considerably more samples, the number of which can be estimated by adopting a combinatorics approach (the branch of mathematics that studies the numbers of different combinations of finite objects). Assuming for simplicity that the frequency of occurrence in each grain size class are represented as either presence or absence (0 or 1), all possible combinations of non-zero classes (i.e., all possible simplified shapes of the grain size distribution) can be calculated from

$$\sum_{k=1}^{n-1} \frac{n!}{k!(n-k)!}$$

where n is the total number of grain size classes (i.e., resolution of dataset), and k is the number of non-zero classes. Here, the number of samples necessary to observe all possible combinations of non-zero classes at least once increases exponentially with the resolution of the dataset (number of grain size classes). This statistical analysis suggests that to fully unravel the highest-resolution laser-derived textural data (in excess of 20 size classes) might require a million-times increase in the number of bottom sediment samples. In essence, results from this study emphasize that data resolution and sea-floor sampling strategies should be intimately linked. Modern instrumentation now makes size analysis quick and reliable (with appropriate care) and data should be collected and measured at the maximum practical resolution, such as the standard output, 32-class size data cited herein. However, data should be reduced for meaningful statistical analysis in accordance with the total sample population.

C–H statistical analysis indicates an optimal solution of 3-textural facies from laboratory-measured grain size data, 6-textural types of sediment cover from bottom photos, but 7 biomass types across the megafaunal assemblages. This result suggests that the relationship between textural facies and benthic biomass is complex, in accordance to other ecological studies e.g., Snelgrove and Butman (1994). However, an alternative explanation could be more closely aligned to sampling bias associated with the assessment of seabed texture. There is a better match between the number of photo-derived textures and biomass categories i.e., texture and benthic biomass might be closely related. An explanation of this outcome may lie in the ability of bottom photographs to capture (sample) a wider range of textural variability than grabs, particularly the coarsest-gravel component (> 2 mm), which are technically difficult sediments to sample in the field, and subsequently sub-sample in the laboratory. This is a relevant topic for future benthic habitat investigations but falls outside the scope offered by the present study.

The advantages of the entropy classification technique for grain size categorization are shown in Fig. 7b, as little overlap exists between the entropy-derived textural facies. Note that based on mean-grain size (or sorting) alone, the boundaries between these three basic textural facies would be gradational and difficult to determine. In this case, the advantages of utilizing all the available particle-size envelope in the textural categorization process are clear. In contrast, a stratigraphic approach shows that there is significant textural complexity between the geological facies, due in part to post-depositional reworking and sampling bias. In this case, a stratigraphic classification does not provide clear discrimination between basic textural types, and hence, basic benthic habitats. Both classification schemes are valid, but have been implemented to address different issues.

7. Conclusions

1. An independent statistical approach pioneered by Calinski and Harabasz (C–H) (1974) offers significant advantages in determining the appropriate number of groups that might exist in any sample population. Used in conjunction with a multivariate extension to information-entropy, grain size populations can be clustered into statistically validated groups.
2. Utilizing a 30-yr legacy of 4-class grain size data (clay, silt, sand, gravel) collected from the Scotian Shelf, Canadian Atlantic continental margin, we show that a traditional stratigraphic approach does not provide clear discrimination between basic textural types, and hence, basic benthic habitats. Considerable improvements in textural zonation are obtained using a combination of information entropy-clustering and C–H technique.
3. Two high resolution 32-class particle size data sets yield a solution that suggests no obvious textural groups exist, contrary to published field-based studies. One possible explanation for this behaviour is that increased resolution leads to an inhe-

rent increase of the within-group variability, which in turn may lead to potentially misleading C–H statistic. Reduction from 32 to 4 broad classes yields a C–H curve that indicates 6 groups are statistically favoured, a result more compatible with field observations.
4. Comparision of sediment grab samples to bottom photographs shows that photos capture (sample) the coarsest-gravel component (>2 mm), which are technically difficult sediments to sample in the field, and subsequently sub-sample in the laboratory, therefore, classification from photos creates more groups.
5. Results from this study emphasize that data resolution and sea-floor sampling strategies should be intimately linked, and to fully unravel high-resolution laser-derived textural data might require a 3–4 order of magnitude increase in the number of bottom sediment samples. Data should be collected at the highest practical resolution, but be reduced to a resolution meaningful for statistical analysis in accordance with the total sample population.

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References

Calinski, T., Harabasz, J., 1974. A dendrite method for cluster analysis. Commun. Stat. 3, 1–27.

Fader, G.B.J. 2004. Regional surficial geology of the Scotian Shelf, Atlantic Ocean, Canada. Geological Survey of Canada Open File Report 4671. Ottawa, Ontario, Canada Natural Resources Canada, Geological Survey of Canada.

Fader, G.B.J., King, L.H., Josenhans, H.W., 1984. Surficial geology of the Laurentian Channel and western Grand Banks of Newfoundland. Marine Sciences, Paper vol. 21. Department of Fisheries and Oceans, Ottawa. 37 pp.

Fader, G.B.J., King, L.H., MacLean, B., 1977. Surficial geology of the eastern Gulf of Maine and Bay of Fundy. Canadian Hydrographic Service, Marine Science Paper 19, Geological Survey of Canada, Paper 76-17, Department of Energy, Mines and Resources, Ottawa, Canada.

Forrest, J., Clark, N.R., 1989. Characterizing grain size distributions: evaluation of a new approach using a multivariate extension of entropy analysis. Sedimentology 36, 711–722.

Full, W.E., Ehrlich, R., Kennedy, S.K., 1983. Optimal definition of class intervals from frequency tables. Part. Sci. Technol. 1, 281–293.

Greene, H.G., Yoklavich, M.M., Sullivan, D., Cailliet, G.M., 1995. A geophysical approach to classifying marine benthic habitats: Monterey Bay as a model. Applications of Side-Scan Sonar and Laser-Line Systems in Fisheries Research. Alaska Fish and Game Special Publication, vol. 9, pp. 15–30. Juneau.

Johnston, R.J., Semple, R.K., 1983. Classification Using Information Statistics: Concepts and Techniques in Modern Geography, vol. 46. Geobooks, Norwich, pp. 157–160.

King, L.H., 1970. Surficial Geology of the Halifax–Sable Island Map-Area, Paper 1. Marine Sciences Branch, Department of Energy, Mines and Resources, Ottawa. 16 pp.

King, L.H, Fader, G.B.J., 1986. Wisconsinan glaciation of the Atlantic continental shelf of southeast Canada. Geol. Surv. Can. Bull. 363 (72 pp.).

King, L.H., MacLean, B., 1976. Geology of the Scotian Shelf. Canadian Hydrographic Service, Marine Sciences Paper 7. Geological Survey of Canada Paper 74-31, 31 pp.

King, L.H., MacLean, B., Fader, G.B., 1974. Unconformities on the Scotian Shelf. Can. J. Earth Sci. 11, 89–100.

Kostylev, V.E., Todd, B.J., Fader, G.B.J., Courtney, R.C., Cameron, G.D.M., Pickrill, R.A., 2001. Benthic habitat mapping on the Scotian Shelf based on multibeam bathymetry, surficial geology and sea floor photographs. Mar. Ecol. Prog., Ser. 219, 121–137.

Kostylev, V.E., Courtney, R.C., Robert, G., Todd, B.J., 2003. Stock evaluation of giant scallop (*Placopecten magellanicus*) using high-resolution acoustics for seabed mapping. Fish. Res. 60, 479–492.

Legendre, P., Ellingsen, K.E., Bjørnbom, E., Casgrain, P., 2002. Acoustic seabed classification: improved statistical method. Can. J. Fish. Aquat. Sci. 59, 1085–1089.

Milligan, G.W., Cooper, M.C., 1985. An examination of procedures for determining the number of cluster in data set. Psychometrika 50, 159–179.

Newell, R.C., Seiderer, L.J., Hitchcock, D.R., 1998. The impact of dredging works in coastal waters: a review of the sensitivity to disturbance and subsequent recovery of biological resources on the sea bed. Oceanogr. Mar. Biol. Ann. Rev. 36, 127–178.

Orpin, A.R., Woolfe, K.J., 1999. Unmixing relationships as a method of deriving a semi-quantitative terrigenous sediment budget, central Great Barrier Reef lagoon, Australia. Sediment. Geol. 129, 25–35.

Orpin, A.R., Haig, D.W., Woofle, K.J., 1999. Sedimentary and foraminiferal facies in Exmouth Gulf, arid tropical northwestern Australia. Aust. J. Earth Sci. 46, 607–621.

Orpin, A.R., Brunskill, G.J., Zagorskis, I., Woolfe, K.J., 2004. Patterns of mixed siliciclastic-carbonate sedimentation adjacent to a large dry-tropics river on the central Great Barrier Reef shelf, Australia. Aust. J. Earth Sci. 51, 665–683.

Pelletier, B.R., 1974. Sedimentary textures and relative entropy and their relationship to the hydrodynamic environment Bay of Fundy system. Offshore Geology of Eastern Canada, Vol. 1, Concepts and Applications of Environmental Marine Geology, Geological Survey of Canada Paper 74-30, pp. 77–95.

Piper, D.J.W., Mudie, P.J., Fader, G.B., Josenhans, H.W., MacLean, B., Vilks, G., 1990. Quaternary geology, Chapter 10. In: Keen, M.J., Williams, G.L. (Eds.), Geology of the Continental Margin of

Eastern Canada, Geological Survey of Canada, Geology of Canada, vol. 2, pp. 475–607.
Porter-Smith, R., Harris, P.T., Anderson, O.B., Coleman, D., Greenslade, D., Jenkins, C.J., 2004. Classification of the Australian continental shelf based on predicted sediment threshold exceedance from tidal currents and swell waves. Mar. Geol. 211, 1–20.
Rumbolt, S.T., Kostylev, V.E., 2004. Geological survey of Canada database of photo and video surveys of the seabed off Nova Scotia; Open File Report 4939, 339 pp.
Semple, R.K., Youngman, C.E., Zeller, R.E., 1972. Economic regionalization and information theory: an Ohio example. Discussion Paper 28. Department of Geography, Ohio State University, Columbus. 64 pp.
Shannon, E., [1948] 1963. Bell System Tech. Jour. 379, 623. Reprinted in: Shannon C.E., Weaver, W. (Eds), The Mathematical Theory of Communication, University of Illinois Press, Urbana, Illinois.
Sharp, W.E., 1973. Entropy as a parity check. Earth Res. 1, 27–30.
Snelgrove, P.V.P., Butman, C.A., 1994. Animal–sediment relationships revisited: cause versus effect. Oceanogr. Mar. Biol. Ann. Rev. 32, 111–177.
Stewart, P.L., Levy, H.A., Hargrave, B.T., 2001. Database of benthic macrofaunal biomass and productivity measurements for the eastern Canadian continental shelf, slope and adjacent areas. Canadian Technical Report of Fisheries and Aquatic Sciences 2336, vi+ 31 p. +A1-6, ISSN 0706-6457.
Todd, B.J., Fader, G.B.J., Courtney, R.C., Pickrill, R.A., 1999. Quaternary geology and surficial sediment processes, Browns Bank, Scotian Shelf, based on multibeam bathymetry. Mar. Geol. 162, 167–216.
Woolfe, K.J., Michibayashi, K., 1995. BASIC entropy grouping of laser-derived grain size data: an example from the Great Barrier Reef. Comput. Geosci. 21, 447–462.
Woolfe, K.J., Larcombe, P., Orpin, A.R., Purdon, R.G., Michaelsen, P., McIntyre, C.M., Amjad, N., 1998a. Controls upon inner-shelf sedimentation, Cape York Peninsula, in the region of 12°S. Aust. J. Earth Sci. 45, 611–621.
Woolfe, K.J., Fielding, C.R., Howe, J.A., Lavelle, M., Lally, J.H., 1998b. Laser-derived particle size characterisation of CRP-1, McMurdo Sound, Antarctica. Terra Antarctica 5, 383–391.
Woolfe, K.J., Larcombe, P., Stewart, L.K., 2000. Shelf sediments adjacent to the Herbert River delta, Great Barrier Reef, Australia. Aust. J. Earth Sci. 47, 301–308.