Combining observations with acoustic swath bathymetry and backscatter to map seabed sediment texture classes: the empirical best linear unbiased predictor

R.M. Lark<sup>a\*</sup>, B.P. Marchant<sup>a</sup>, D.Dove<sup>b</sup>, S.L. Green<sup>b</sup>, H. Stewart<sup>b</sup>, M. Diesing<sup>c</sup>

<sup>a</sup>British Geological Survey, Keyworth, Nottingham, NG12 5GG, <sup>b</sup>British Geological Survey, Murchison House, Edinburgh, EH9 3LA, <sup>c</sup>Centre for Environment, Fisheries and Aquaculture Science, Pakefield Road, Lowestoft, Suffolk NR3 30HT

# Abstract

3 Seabed sediment texture can be mapped by geostatistical prediction from limited

4 direct observations such as grab-samples. A geostatistical model can provide local

estimates of the probability of each texture class so the most probable sediment

class can be identified at any unsampled location, and the uncertainty of this pre-

7 diction can be quantified. In this paper we show, in a case study off the northeast

s coast of England, how swath bathymetry and backscatter can be incorporated into

<sup>9</sup> a geostatistical linear mixed model (LMM) as fixed effects (covariates).

Parameters of the LMM were estimated by maximum likelihood which allowed us to show that both covariates provided useful information. In a cross-validation, each observation was predicted from the rest using the LMMs with (i) no covariates, or (ii) bathymetry and backscatter as covariates. The proportion of cases in which the most probable class according to the prediction corresponded to the observed class was increased (from 58% to 65% of cases) by including the covariates which also increased the information content of the predictions, measured by the entropy of the class probabilities. A qualitative assessment of the geostatistical results shows that the model correctly predicts, for example, the occurrence of coarser sediment over discrete glacial sediment landforms, and muddler sediment in relatively quiescent,

<sup>\*</sup>Corresponding author: E-mail address: mlark@bgs.ac.uk (R.M. Lark).

localized deep water environments. This demonstrates the potential for assimilating geophysical data with direct observations by the LMM, and could offer a basis for a routine mapping procedure which incorporates these and other ancillary information such as manually-interpreted geological and geomorphological maps.

24 25

# 1. Introduction

Mapping benthic habitats is crucial for underpinning decision-making concerning 27 management of the seabed. To encourage good practice and to ensure comparability across environmental and political boundaries, many practitioners use the hierarchical European Nature Information System (EUNIS) habitat classification scheme (e.g., Connor et al., 2006). The foundation of the EUNIS classification for the seabed is the seabed substratum type, because of the influence this has on the occurrence and abundance of benthic flora and fauna. Seabed habitats are principally split into rock and other hard substrata on the one hand, and sediment habitats on the other. Rock habitats have been identified as important for conservation due to their high biodiversity (e.g., Evans et al., 2015). However, they only account for a very limited area of seabed, which is typically dominated by sediment over large parts of the con-37 tinental shelves. Mapping the distribution of seabed sediment classes can therefore serve as a proxy for regional benthic habitats (e.g., Kostylev et al., 2001; Howell, 2010; McGonigle and Collier, 2014). The distribution of seabed sediments is also of immediate interest to any industry (e.g., offshore wind, oil and gas) which seeks 41 to install seabed infrastructure, where specific considerations may include sediment mobility, constraints on pile design, or pollutant dispersal (International Association of Oil & Gas Producers, 2013). 44 The acquisition of seabed sediment samples is most commonly achieved by grab 45 sampling, and samples are characterized through particle size analysis (PSA) using the 'Wentworth' textural classification (Wentworth, 1922). When mapping seabed sediment distribution, geologists commonly employ the Folk classification scheme (Folk, 1954) as it provides a useful indication of the energy of the seabed environment, but within the EUNIS habitat mapping classification the Folk scheme is simplified into only four textural classes which can be identified from the proportions of gravel, sand and mud size fractions among the mineral particles of the sediment (Long, 2006). The definitions of these classes are shown in Fig. 1 on the ternary diagram for gravel, sand and mud.

Lark et al. (2012) explored the use of geostatistical methods to predict the distribution of gravel, sand and mud fractions directly from point observations by compositional cokriging. However, this exploits only the spatial dependence of the variation of particle size fractions as shown by the data, and does not incorporate other types of relevant information. One example is data from swath bathymetry surveys. Both the bathymetry, and the associated intensity of the backscatter signal from the seabed, are informative about sediment texture (e.g., Goff et al., 2004; Fonseca et al., 2009).

Commonly, bathymetry and backscatter data are used to map the distribution 63 of textural classes by expert interpretation. This interpretation is conducted in the light of the evolution of the seabed. When extrapolating the sample point data according to the geographically continuous acoustic data, the expert interpreter may consider, for example, how the interplay of the pre-existing geological substrate is modified over multiple climatic and environmental timescales (e.g., glaciation); and how the evolving seabed geomorphology is further impacted upon by active 69 sedimentary, hydrodynamic, or even biological processes. There are many examples of such interpretative studies (e.g., Hughes Clarke et al., 1996; Kostylev et al., 2001; 71 Glynn et al., 2015). Expert interpretation, however, is demanding of time. There is also an element of subjectivity in the results as they depend on judgements which may differ between individuals. Because of this, there has been considerable interest in developing quantitative techniques to establish predictive relationships between acoustic data and sediment properties (see review by Brown et al., 2011).

There are two general quantitative approaches. The first uses physical models of 77 the backscattering of an acoustic signal by material on the seabed. At any location the sediment properties are found that give the best match between the predicted and observed backscatter (e.g., Sternlicht and de Moustier, 2003; Snellen et al., 2011). A second approach uses statistical predictive relationships. These may be 81 semi-empirical, a predictive function with a physical interpretation is fitted statistically to observed data on sediment texture and the acoustic signal (e.g., Endler et al, 2015). Other statistical methods that have been applied include multivari-84 ate clustering (e.g., Anderston et al, 2002), clustering on multifractal properties of the time-dependent backscatter (Haris and Chakraborty, 2014), decision trees (e.g., Dartnell and Gardner, 2004), artificial neural networks (e.g., Marsh and Brown, 87 2009) and random forests (e.g., Lucier et al., 2013).

In a comparative study by Diesing et al. (2014) a range of mapping approaches was applied for interpretation of seabed sediments based on acoustic data (swath bathymetry, backscatter and derivatives of bathymetry such as rugosity which is 91 a measure of high-frequency roughness) along with PSA samples. The approaches undertaken included expert interpretation, geostatistics (cokriging), object-based image analysis (OBIA) and random forests. In this case, the geostatistical method did not incorporate the acoustic data, whereas they were used by the machine learning, OBIA and expert interpretation techniques. However, these do not account explicitly for the spatial distribution of the observations, nor of the spatial depen-97 dencies among the data (although the more desirable properties of machine-learning methods such as random forests depend on the assumption that the observations are independent). Diesing et al. (2014) compared their results for prediction using 100 acoustic data with the direct application of cokriging, as described by Lark et al. 101 (2012). They found that a pixel by pixel comparison between the outputs resulted 102 in agreements of between 68.1% and 73.1% for the cokriging method when compared with the mapped outputs from the other techniques. There was a marked difference between this method and those which utilised the acoustic data, with the major differences resulting from the less frequently occurring sediment classes.

In this paper we consider the possibility of combining linear models for the 107 relationship between particle size distribution and variables derived from acoustic 108 data with the cokriging procedure to account for the remaining unexplained vari-109 ation. This is done by fitting a linear mixed model (LMM) for the (appropriately 110 transformed) particle size distribution of sediment with fixed effects (covariates) the bathymetry and backscatter from the acoustic survey, and a suitable linear model 112 of coregionalization for the residuals. The prediction conditional on this model is 113 the empirical best linear unbiased predictor with the mean vector of the dependent 114 variables a function of the covariates. We compare this result with the ordinary 115 cokriging method in which the mean vector is assumed to be constant. 116

#### 117 2. Methods

- 118 2.1 The statistical model
- 2.1.1 Compositional data and their treatment

Seabed sediment texture classes are defined according to the proportions by mass of gravel, sand and mud in the sediment on the logarithmic Wentworth scale (Wentworth, 1922). The size classes are exhaustive, and so the proportions of gravel, sand and mud necessarily sum to one. This makes the variate a composition (Aitchison, 1986) which is constrained to a distribution on the two-dimensional simplex, and which can be plotted as a ternary diagram.

The compositional nature of data such as those on sediment particle sizes must
be accounted for in analysis. The problem is that, because the gravel, sand and mud
proportions sum to one, they cannot vary jointly like other multivariate data sets,
and spurious correlations can emerge between variables. The methods to deal with
this problem that Aitchison (1986) proposed are based on taking ratios between
compositional variables. Whereas sand and mud proportions cannot vary indepen-

dently (if, for example, we know that the mud proportion is 0.7 then we know that
the sand proportion is less than or equal to 0.3), their respective ratios to the gravel
proportion are not so constrained. These ratios are generally transformed to logarithms to make an assumption of a joint normal distribution plausible. These are
called the additive log-ratios of the compositional variables.

Lark et al. (2012) used compositional cokriging, as described by PawlowskyGlahn and Olea (2004), to predict seabed sediment texture by ordinary cokriging
of the additive log-ratios. The additive log-ratio (ALR) transform can be applied
to an m-part composition to create m-1 new variables which are not constrained
onto a m-1-dimensional simplex but can be regarded as an unconstrained m-1dimensional variate.

In the case of a three-variate compositional random variable  $\mathbf{Z} = \{Z_1, Z_2, Z_3\}$  a corresponding two-dimensional ALR variate is  $\mathbf{Y} = [Y_1, Y_2]^{\mathrm{T}}$ , where

$$Y_1 = \ln \frac{Z_1}{Z_3},$$
  
 $Y_2 = \ln \frac{Z_2}{Z_3}.$  (1)

Note that the selection of a variable from the compositional variate to serve as the denominator of the log-ratio does not affect the final outcome of analyses (Pawlowsky-Glahn and Olea, 2004). The ALR transform can be inverted:

$$\mathbf{Z} = \left\{ \frac{\exp(Y_1)}{1 + \exp(Y_1) + \exp(Y_2)}, \frac{\exp(Y_2)}{1 + \exp(Y_1) + \exp(Y_2)}, \frac{1}{1 + \exp(Y_1) + \exp(Y_2)} \right\}^{\mathrm{T}}, (2)$$

, where the superscript T indicates the transpose of the matrix.

2.1.2 The linear mixed model for compositional data

Lark et al. (2012) used cokriging of the ALR-transform of the particle size composition. They sampled the prediction distribution of the ALR-transformed variate at the nodes of a prediction grid to estimate the probability at each node that each of the EUNIS sediment texture classes occurred. In this paper we extend this methodology to include bathymetry and backscatter as predictive covariates.

This is done in the linear mixed modelling framework following the methods of Marchant and Lark (2007).

Consider a simple case where a two-dimensional ALR variate,  $\mathbf{Y}$ , is to be modelled as a linear function of some covariate X. We have n collocated observations of the two ALR variables which we denote by the  $n \times 1$  vectors  $\mathbf{y}_1$  and  $\mathbf{y}_2$ , let  $\mathbf{x}$  denote the  $n \times 1$  vector of corresponding observations of the covariate, and let  $\mathbf{1}_n$  denote a  $n \times 1$  vector of ones. The LMM for  $\mathbf{Y}$  is

$$\begin{bmatrix} \mathbf{y}_1^{\mathrm{T}} \\ \mathbf{y}_2^{\mathrm{T}} \end{bmatrix} = \begin{bmatrix} \alpha_1 & \beta_1 \\ \alpha_2 & \beta_2 \end{bmatrix} \begin{bmatrix} \mathbf{1}_n^{\mathrm{T}} \\ \mathbf{x}^{\mathrm{T}} \end{bmatrix} + \begin{bmatrix} \boldsymbol{\eta}_1^{\mathrm{T}} \\ \boldsymbol{\eta}_2^{\mathrm{T}} \end{bmatrix} + \begin{bmatrix} \boldsymbol{\varepsilon}_1^{\mathrm{T}} \\ \boldsymbol{\varepsilon}_2^{\mathrm{T}} \end{bmatrix}. \tag{3}$$

There are many terms in this equation, and we define and explain them in the 162 following paragraphs. First,  $\alpha_1$  and  $\beta_1$  are a constant and linear regression coefficient 163 for variable  $Y_1$ , and  $\alpha_2$  and  $\beta_2$  are corresponding coefficients for  $Y_2$ . These are known 164 as fixed effects in the LMM. The terms  $\eta_1$  and  $\eta_2$  are spatially correlated random 165 effects of mean zero, which we assume conform to a linear model of coregionalization 166 (LMCR, Journel and Huijbregts, 1978). Let us denote some element of  $\eta_i$ , where 167  $i \in \{1,2\}$  by  $\eta_i(\mathbf{s})$  where  $\mathbf{s}$  is a vector with the coordinates of the observation in space. Under the LMCR the covariance of any two observations separated spatially 169 by a lag vector  $\mathbf{h}$ :  $\eta_i(\mathbf{x}), \eta_i(\mathbf{x} + \mathbf{h})$ , is assumed to depend only on the lag vector and 170 is given by 171

$$K_{i,j}(\mathbf{h}) = \sum_{k=1}^{s} c_k^{i,j} \rho_k(\mathbf{h}), \tag{4}$$

where there are  $s \ge 1$  independent additive components in the model, the terms  $c_k^{i,j}$  are variances and covariances that constitute a positive-definite covariance matrix for any k and  $\rho_k(\mathbf{h})$  is a spatial correlation function. In this study we assume that the correlation function is isotropic (it depends on the lag distance,  $|\mathbf{h}|$ , not the direction), and can be described by the function due to Matérn (Stein, 1999):

$$\rho(\mathbf{h}) = \frac{1}{2^{\nu-1}\Gamma(\nu)} \left(\frac{2\nu^{\frac{1}{2}}|\mathbf{h}|}{\phi}\right)^{\nu} \mathcal{K}_{\nu} \left(\frac{2\nu^{\frac{1}{2}}|\mathbf{h}|}{\phi}\right), \tag{5}$$

where  $\phi$  is a distance parameter,  $\nu$  is a smoothness parameter and  $\mathcal{K}_{\nu}$  is a modified

Bessel function of the second kind of order  $\nu$ . In this study we consider only one spatially correlated component in the LMCR.

Under this model, and the assumption of a normal distribution, the terms  $\eta_1$  and  $\eta_2$  are therefore entirely characterized by the variances and covariance  $c_1^{1,1}, c_1^{2,2}$  and  $c_1^{2,1}$  and the parameters  $\phi$  and  $\nu$  of the Matérn correlation function.

Each term  $\varepsilon_1$  and  $\varepsilon_2$  in Eq. (3) is a zero-mean independently and identically dis-183 tributed random effect, although there may be a non-zero cross-correlation. Under 184 the assumption of normality, these terms are entirely characterized by their variances 185 and covariance, which we denote by  $c_0^{1,1}, c_0^{2,2}$  and  $c_0^{2,1}$ . These terms are spatially un-186 correlated, and so represent components of the variation of our variables which are 187 either not spatially-dependent, or which are spatially dependent at scales too fine to 188 be resolved by the sampling of the variables. This component of the LMM is called 189 the 'nugget', a term inherited from the origin of geostatistics in mining geology. 190

If the parameters of the LMM are known, then we may use them to predict values 191 of the variables  $Y_1$  and  $Y_2$  at unsampled sites where the covariate X is known. 192 There are two components to the prediction. The first may be thought of as a 193 regression-type prediction, depending on the value of the covariate and the fixed 194 effects parameters  $\alpha_1$ ,  $\alpha_2$ ,  $\beta_1$  and  $\beta_2$ . The second component is a cokriging-type 195 prediction of the random effects  $\eta_1$  and  $\eta_2$ , and depends on the parameters of the 196 LMCR. The predictions of  $Y_1$  and  $Y_2$  have unknown errors at any site. The variance 197 and covariance of these errors can be computed from the LMM. 198

2.1.3 Estimation of model parameters and model selection

In practice, the parameters of the LMM are unknown and must be estimated from data. Under the assumption of normally distributed random effects this can be done by maximum likelihood (ML), although this results in biased estimates of the parameters of the random effects because the fixed effects coefficients are nuisance parameters. An alternative is to use residual maximum likelihood (REML) due to Patterson and Thompson (1971) which is ML estimation applied to a projection of

the data in which the fixed effects have known zero mean. Once REML estimates of the random effects parameters are obtained then the fixed effects parameters can be estimated by weighted least squares. Marchant and Lark (2007) describe the use of REML to estimate LMCR parameters. REML reduces bias, and so we use it here to estimate model parameters to use in prediction.

One may use ML or REML followed by generalized least squares to estimate 211 the random and fixed effects coefficients of any proposed LMM. In many contexts, 212 including this study, we need to evaluate the evidence for including particular fixed 213 effects. One might ask, for example, whether a model with bathymetry and backscat-214 ter as fixed effects is to be preferred to one with a constant mean as the only fixed 215 effect. Equally one might ask whether adding backscatter to a model which includes 216 bathymetry is justified by the available data. These decisions are based on the ev-217 idence provided by the maximized likelihood for the fitted models. However, two 218 important points must be noted. 219

First, a pair of models with different fixed effects (e.g., a model with no covariates so that the overall mean is the only fixed effect, and a model with acoustic backscatter) can be compared on the likelihood, but not on the residual likelihood. For purposes of selecting a fixed effects structure we therefore fitted models by ML, and then used REML to estimate the parameters of the selected model.

Second, adding fixed effects to a model cannot result in a reduction in the maximized likelihood (since, at worst, the coefficient of the new fixed effect can go to
zero, leaving the likelihood unchanged). Usually the likelihood is increased by adding
new fixed effects. This does not mean that the additional covariates are genuinely
informative. One standard criterion used to assess whether additional covariates
in a model are justified in terms of improved predictive value is Akaike's information criterion (AIC) (Akaike, 1973). If  $\ell$  is the natural logarithm of the maximized
likelihood for the fit of a model with P predictors then the AIC is computed as

$$A = 2P - 2\ell. (6)$$

One selects from a set of models the one for which AIC is smallest. The criterion
can therefore be thought of as based on the goodness of fit, with a penalty for model
complexity. By selecting from a set of models the one with the smallest AIC one
minimizes the expected information loss through the selection decision (Verbeke and
Molenberghs, 2000).

# 2.1.4 Prediction from the model

Estimated parameters of the LMM can be used to obtain predictions at unsam-239 pled sites. This prediction is called the empirical best linear unbiased prediction 240 (E-BLUP) (Stein, 1999). Along with the E-BLUP one can also obtain its covariance 241 matrix, the variances and covariance of the prediction errors. For more details of the 242 estimation and prediction procedure, the reader is referred to Marchant and Lark 243 (2007). The E-BLUP and its covariance matrix together define the prediction distri-244 bution of the modelled variables at the unsampled site. The prediction distribution 245 represents the uncertainty about the actual values of these variables at that site. 246

Given the E-BLUP and its covariance matrix at any location, one can simulate values of ALR-transformed gravel, sand and mud content from the prediction distribution. Any simulated set of values can be back-transformed to the original compositional variate by Eq. (2). One may use this sample to estimate properties of the unknown composition at the prediction site, such as the distribution of one of its components. This was done by Lark et al. (2012) in the ordinary cokriging case.

#### 253 2.2 Geological setting

The study area is located approximately 11 km off the Northumberland coast in northeast England and covers an area of approximately 705 km<sup>2</sup> (Fig. 2) with depth of water varying between 50 and 110 m. It was chosen because it was expected to show variability in seabed geomorphology, bathymetry, and associated seabed sediment distribution, providing a suitable environment to test the geostatistical modelling. This variability in seabed character is a function of the complex geological history preserved at seabed including the presence of bedrock at or near-seabed,

glacial landforms, and mobile sediment bedforms. The high-relief bathymetry also allows for distinct hydrodynamic conditions, as where local bathymetric deeps preserve mud accumulations.

Streamlined glacial landforms, overlying the bedrock, are prominent at the seabed 264 of the study area and reflect ice stream pathways associated with the British ice sheet 265 (BIS) over the last glacial cycle (Clark et al., 2012) (see the bathymetry of the area 266 in Fig. 3a). While our understanding of the extent, timing and dynamics of the 267 glaciation within this sector of the North Sea basin is only recently being improved 268 (Graham et al., 2011; Stewart et al., 2013), the survey area lies just offshore of the 269 projected flow path of the well-described onshore 'Tweed ice stream' (e.g., Everest et 270 al., 2005), and south of the impinging Forth ice stream (Stewart et al., 2013). These 271 streamlined features are interpreted as subglacial landforms elongated parallel to the 272 flow of a palaeo-ice stream (e.g., Stokes and Clark, 2001), and are expected to com-273 prise subglacial till with notable coarse and overconsolidated clay sediment fractions 274 (Gatliff et al., 1994; Stokes et al., 2011). Following the last glacial maximum, marine 275 transgression and flooding of the North Sea brought the re-establishment of marine-276 based erosional and depositional processes. Across the survey we observe series of 277 sinuous, sharp-crested waves interpreted as mobile sediment bedforms. These modern, frequently sand-dominated features are common in the North Sea, and reflect 279 local hydrodynamic conditions and sediment availability (Huntley et al., 1993). 280

# 281 2.3 Data

The bathymetry data were acquired in February–March 2012 in accordance with specifications of the International Hydrographic Organization (2008) for Order 1a, using a Reson 7125 multibeam echosounder aboard the contracted survey vessel MV Neptune. All depth soundings acquired by the multibeam have been reduced to chart datum using a vertical offshore reference frame (VORF) offset value for the centre of the site. The backscatter data were processed with Geocoder software as implemented in Caris HIPS & SIPS. The bathymetry and backscatter values are

shown in Fig. 3a and 3b respectively.

The sediment samples were acquired by the RV Cefas Endeavour over March, 290 2012 with a 0.1-m<sup>2</sup> Hamon grab, concurrent with the geophysical survey. Sample 291 locations were pre-determined according to anticipated distribution of broadscale 292 habitats based on legacy British Geological Survey (BGS) seabed sediment maps. 293 Discrete samples from 75 stations were collected within the region where swath 294 bathymetry and backscatter data had been acquired. The samples were collected at 295 a variable spacing of approximately 3 km on average, and sub-sampled for PSA. The 296 positions of the grab-samples are superimposed on Fig. 3a. Legacy BGS sediment 297 samples also exist within the survey area but these were not incorporated due to 298 concerns with positional accuracy, as they were acquired prior to the use of satellite 299 Global Positioning Systems. 300

The bathymetry and backscatter data are accurate to 2-m grid resolution, but for 301 the purposes of this study were sub-sampled to a 50-m grid spacing (the resolution of 302 the point observations was unchanged but the grid was thinned). This was to reduce 303 the processing requirements for mapping. In principle the mapping could be done 304 on the full resolution data, but it was decided to use a coarser grid because of the 305 relatively sparse distribution of grab-samples. Co-registered bathymetry (metres) 306 and backscatter (decibels) values were extracted at each grab sample location to be 307 used as input for the geostatistical model. 308

#### 309 2.4 Analysis

310 2.4.1 Exploratory data analysis and ALR-transformation

In section 2.1 the ALR transform was introduced in both general and formal terms. As was noted, Pawlowsky-Glahn and Olea (2004) show that the results of cokriging from ALR-transformed values of a compositional variate do not depend on the initial selection of a component of the composition to serve as the denominator of the log ratio. In other words, one might work with the log-ratios of sand to mud and gravel to mud, or the ratios of mud to sand and gravel to sand etc. In this study we

used the proportion of gravel as the numerator and computed transformed variables
that we denote ALR-Sand and ALR-Mud. Exploratory statistics showed that some
of the samples had zero gravel content (Table 1). The ALR transform is not defined
in this case. As in the previous study by Lark et al. (2012) we imputed non-zero
values for compositions with zeroes, following the method of Martín-Fernandéz and
Thió-Henestrosa (2006), and setting zero values to a small value (0.005) less than the
smallest non-zero value in the data before renormalizing the affected compostion.

2.4.2 Model fitting and selection

Because of the skewness of the ALR-transformed variables (Fig. 5) a Box-Cox transformation was incorporated into the LMM. Under the Box-Cox transformation the modelled variable is z where y is the observed variable (ALR-Mud or sand here), and where

$$z = \frac{y^{\lambda} - 1}{\lambda} \quad \lambda \neq 0,$$
  
=  $\ln(y) \quad \lambda = 0.$  (7)

Note that if  $\lambda=1$  the transformation is just a linear offset. The parameter  $\lambda$  is estimated by ML along with the other parameters of the LMM as described in section 2.1.

Linear mixed models of the form of Eq. (3) were first fitted by maximum likelihood with ALR-Sand and ALR-Mud. In the simplest model there was no covariate
so, in effect, the first term on the right-hand side of Eq. (3) was reduced to a vector
with two constants, the overall mean of ALR-Sand and ALR-Mud, respectively. We
considered a model with acoustic bathymetry as the single covariate, and one with
acoustic backscatter as the single covariate. We also considered a model with both
acoustic variables as covariates. We chose between these alternative models on the
basis of the AIC (Eq. 6) as described in section 2.1.3 above.

Having selected among the alternative models fitted by ML, we refitted the selected model by REML. We also used REML to fit the LMM with overall mean the only fixed effects. This is for comparison with a model in which the acoustic

343 data are exploited.

344 2.4.3 Cross validation

Prior to mapping classes with the selected model we undertook two linked validation tests. The first is a test of the LMM to ensure that the E-BLUP based on it
gave plausible predictions of the ALR-transformed PSA data, and that the prediction distributions gave a valid measure of uncertainty. The second was an evaluation
of the predictions of sediment texture class obtained from the E-BLUP.

In the previous study by Lark et al. (2012) we used a witheld subset of the data 350 to evaluate the cokriging predictions. In this study the total number of sites available 351 was too small to justify this procedure. For purposes of comparison of predictions 352 with and without the use of the acoustic data, we used a cross-validation procedure. 353 In cross-validation each data point was excluded from the data in turn and the E-354 BLUP and its covariance matrix at the location of the excluded data point were 355 computed. Each data value can therefore be compared with its E-BLUP computed 356 from the remaining data. 357

The first analyses on the cross-validation outputs are to validate the fitted model.

Each value of ALR-Sand and ALR-Mud in the data set was compared with the crossvalidation prediction. If the observed value of ALR-Sand at location  $\bf s$  is denoted
by  $y_{\rm sand}(\bf s)$  and the E-BLUP is  $\tilde{Y}_{\rm sand}(\bf s)$ , then the squared prediction error is

$$\left\{ y_{\text{sand}}(\mathbf{s}) - \tilde{Y}_{\text{sand}}(\mathbf{s}) \right\}^2$$
 (8)

and the standardized squared prediction error is

$$\frac{\left\{y_{\text{sand}}(\mathbf{s}) - \tilde{Y}_{\text{sand}}(\mathbf{s})\right\}^{2}}{\sigma_{\text{sand}}^{2}(\mathbf{s})},\tag{9}$$

where  $\sigma_{\rm sand}^2(\mathbf{s})$  is the prediction error variance of ALR-Sand at location  $\mathbf{s}$ . This is an element of the covariance matrix of the E-BLUP, referred to above. Since the prediction error variance is the expected squared error of the prediction, the expected value of the standardized squared prediction error is 1.0. The median of the standardized squared prediction errors is a diagnostic statistic for the LMM. If the parameters of the random effects are correct, and the prediction errors are normal, then the expected median is 0.455.

The second set of analyses were to evaluate the predictions of sediment texture 370 class. We are interested in mapping the four broad sediment texture classes of the 371 EUNIS habitat classification, 'Coarse', 'Mixed', 'Mud and Sandy Mud', 'Sand and 372 Muddy Sand', shown on the ternary diagram in Fig. 1. These classes underpin 373 marine habitat mapping (Long, 2006). Lark et al. (2012) showed how this could 374 be done with the ordinary cokriging predictions of ALR-transformed particle size data by sampling from the prediction distribution at prediction sites. This is done 376 by using a random number generator to generate a random pair of values for ALR-377 Sand and ALR-Mud with means equal to the corresponding E-BLUP and covariance 378 matrix equal to the E-BLUP error covariance matrix. The pair of simulated values 379 is then back-transformed to the simplex space of the sand-mud-gravel composition 380 and the corresponding texture class is identified. By repeating this many times one 381 may estimate the probability of each class. This was done for each cross-validation 382 site. If a total of N samples is drawn from the probability distribution for location 383 s, and  $n_i(s)$  of the samples correspond to class i, then the estimated probability that 384 the *i*th class occurs at location s is 385

$$\widehat{p}_i(\mathbf{s}) = \frac{n_i(\mathbf{s})}{N}.$$
(10)

At site s the best prediction of the texture class, in the sense of the prediction most likely to be correct, is the class for which the estimated probability,  $\hat{p}_i(\mathbf{s})$ , is largest. We evaluated these predictions over all sites. Over all sites the known class may be compared with the most probable class (the class to which most of the samples from the prediction distribution belong) in an error matrix. Various measures of the success of the prediction can be computed from this matrix (Lark, 1995). The first is the overall purity of the mapped legend classes, estimated by the proportion of cross-validation sites in which the observed class is also the most probable class. For each class, one may compute a separate purity, estimated by the proportion of those cross-validation sites at which the class of interest is the most probable where this class is the one actually observed. One may also compute the representation of each class. The representation of a class is estimated by the proportion of those cross-validation sites where that class is observed at which it is the most probable class according to the sample from the prediction distribution.

The overall purity of the prediction should be compared with two benchmark 400 values. One is the proportion of all sites in the most frequent class (since that is 401 the overall purity of a notional map in which all sites are allocated to the most 402 frequent class). The second is the probability of correctly identifying the class at 403 a site by a random guess where the probability of guessing class i is equal to the 404 overall proportion of the area of interest in class i. We estimated the probability 405 of guessing each class from the proportion of the sample data in that class. Let  $\hat{\pi}_i$ 406 be the proportion of the sample in the ith out of I classes. The estimate of the 407 probability of correctly identifying the class by a random guess is then 408

$$\sum_{i=1}^{I} \widehat{\pi}_i^2. \tag{11}$$

The overall purity, class purity and class representations are based only on the 409 most-probable mapped class at each validation location. This is the best predic-410 tion at a site, but the output of the procedure presented in this paper also gives 411 an indication of how confident we can be in the prediction because probabilities are 412 computed for all classes. Consider two locations at which the probabilities for the four sediment classes are, respectively,  $\{0.5, 0.2.0.25, 0.05\}$  and  $\{0.8, 0.1.0.05, 0.05\}$ . 414 In both cases the first class is the most probable, but we are more certain about 415 the allocation in the second case. In the context of this study we are interested in 416 whether the confidence in the predicted texture class, as measured by the class prob-417 abilities, is improved by including bathymetry and backscatter in the LMM. Two 418 such sets of probabilities can be compared by computing their respective entropies. 419 If  $\pi_i$  is the probability of the ith out of m classes at some location, then the entropy of the set of probabilities over all classes is:

$$\mathcal{E} = -\sum_{i=1}^{m} E_i, \tag{12}$$

422 where

423

$$E_i = \pi_i \log \pi_i, \quad \pi_i > 0$$
$$= 0. \qquad \pi_i = 0$$

If natural logarithms are used then the entropy is measured in nats. The en-

tropy for the two example sets of probabilities given above are 1.16 and 0.71 nats 424 respectively. The entropy is larger for the more uniform ensemble of probabilities 425 where the uncertainty is larger. We call the entropy of the set of probabilities, com-426 puted from the E-BLUP prediction distribution at a site, the prediction entropy at 427 that site. As a measure of the uncertainty of the predictions with and without the 428 bathymetry and backscatter data, we computed the mean prediction entropy for 429 each method over the cross-validation points. We also computed the entropy for the 430 overall proportions of all the classes. The comparison between this class entropy 431 and the mean prediction entropy is a measure of how much additional information 432 the E-BLUP provides. 433 Note that the mean entropy of a set of class predictions is computed without 434 reference to whether the most-probable class is the observed class at these sites. It is 435 therefore a measure of the 'internal' confidence of the prediction, i.e., the extent to 436 which the computed class probabilities indicate one very likely class at that site, or 437 several classes with similar probabilities. In general one might expect map purities 438 and representations to be improved by the inclusion of a covariate in the LMM which 439 reduces the mean entropy, but in principle these two sets of statistics could show 440 opposing trends. It is therefore necessary to compute both sets of statistics for a full evaluation of a predictive model and to compare them both between models. 442

443 2.4.4 Mapping

The prediction distribution from the E-BLUP was evaluated at each node of

the bathymetry/backscatter 50-m grid using the LMM with no covariates and the LMM with covariates selected from bathymetry and backscatter according to AIC, as described in the previous section. By numerical integration, the probability of each EUNIS sediment class was evaluated at each node. On this basis the most probable class could be identified and mapped, as could the probability of any one class. The entropy of the set of probabilities at each node was evaluated using Eq. 12.

#### 452 3. Results

472

### 3.1 Exploratory statistics

Table 1 shows summary statistics of the data from PSA expressed as percent-454 ages. Fig. 4 shows the ALR-transformed sand and mud data (with gravel as the 455 denominator) expressed as quartiles (divisions of the range of values which partition 456 the data into four equal-sized subsets). The figure shows the spatial dependence of the PSA data; neighbouring observations tend to be more similar with respect to 458 both variables than observations which are further apart in space. This is encour-459 aging because such spatial dependence is captured by the LMM and provides the 460 basis for the spatial prediction. In Fig. 5 the histograms of the ALR-Sand and mud 461 contents are shown, and scatter plots of these two variables and of the bathymetry 462 and backscatter values at the grab-sample locations. Note that both ALR-Sand 463 and ALR-Mud have skew distributions, despite the log-transformations. This is the 464 rationale for the inclusion of the Box-Cox transformation in the further analysis 465 (Eq. 7). ALR-Mud and ALR-Sand are strongly correlated. Because this correlation 466 appears after the ALR transform we can be confident that it is not a spurious corre-467 lation due to compositional effects (Pawlowsky-Glahn and Olea, 2004). It appears 468 that, in this particular setting, the sandy and muddy sediments have comparable 469 spatial distributions relative to gravel. This can also be seen in Fig. 4, the spatial 470 distribution of the quartiles of ALR-Mud and ALR-Sand are very similar. 471

The bathymetry and backscatter values also show a strong correlation, which

can also be seen in Figs. 2 and 3, the backscatter is smallest from deeper locations.

This correlation is of interest because it is possible that one of these variables could

be regarded as a proxy for the other, and that adding both to the LMM is therefore

not justified. This is tested by the use of AIC for model selection.

In Fig. 6 are shown scatter-plots of the ALR-transformed sand and mud content 477 against both backscatter and bathymetry. The correlation coefficients are also shown 478 on each plot. Note that there is a moderate to strong correlation between both ALR-479 Mud and ALR-Sand and backscatter, and a moderate correlation in both cases with 480 bathymetry. This is encouraging because it suggests that either or both covariates 481 may provide useful information for statistical prediction of the sediment data as 482 fixed effects in the LMM. Note that there is more scatter in these plots where the 483 backscatter is small (deeper sites). This potentially introduces some kurtosis (heavy 484 tails) into the distribution of the random component of the LMM, which is another 485 advantage of including the Box-Cox transformation. 486

# 487 3.2 Model-fitting

Table 2 presents the statistics of the LMMs. Note that the AIC is smallest for 488 the model with bathymetry and backscatter both included as fixed effects. This is 489 interesting because it shows that both covariates together provided more information 490 about sediment composition than did either covariate separately, despite their strong 491 correlation. Because the Box-Cox transformation differs between the models, we 492 may not compare their variance components directly. However, it is interesting to 493 note that in the model with no covariates, the correlated variances and covariances 494 in the model  $(c_1^{\rm S,S},\ c_1^{\rm M,M}$  and  $c_1^{\rm S,M})$  are all notably larger than the corresponding 495 nugget variances and covariances  $(c_0^{\mathrm{S,S}},\,c_0^{\mathrm{M,M}})$  and  $(c_0^{\mathrm{S,M}})$ . However, in the model with 496 bathymetry and backscatter included as covariates, the position is reversed, and 497 the nugget components of variance are the largest. This indicates that much of 498 the long-range spatial variability that the relatively sparse grab-sampling resolves is accounted for by the covariates. 500

One may also compute the correlation between the coregionalized random com-501 ponents for ALR-Sand and ALR-Mud in the LMM. In this case there are two compo-502 nents, one of which is the nugget and the other the spatially correlated component. 503 In the case of the model with no covariates this 'structural correlation' is 0.98 for 504 the nugget component and 0.96 for the spatially correlated component of the model, 505 showing that these particle size components are similarly strongly correlated at 506 both fine and coarse spatial scales. By contrast, the nugget and spatially correlated 507 structural correlations for the random terms, in the model with bathymetry and 508 backscatter included as covariates, are 0.96 and 0.75 respectively. This shows that 509 the fine-scale variability in ALR mud and sand not accounted for by the covariates 510 remain strongly correlated, but that the coarser-scale variation is somewhat less 511 strongly correlated. In other words, the covariates account for coarse-scale sources 512 of variation which affect both mud and sand content of the sediment similarly, and 513 the patterns of coarse-scale variation which remains unaccounted for by these covari-514 ates are similar for the two variables, but rather less similar than the corresponding 515 fine-scale variation. 516

Figure 7 shows the histograms of the cross-validation error for both variables 517 under both LMM. In all cases, the errors have a symmetrical distribution which 518 resembles a normal distribution. Table 3 shows the cross-validation results for Box-519 Cox transformed ALR-Sand and mud content. The mean square error for both 520 ALR-Sand and ALR-Mud (Eq. 8) is notably reduced by including bathymetry and backscatter as covariates. Note that in all cases the mean standardized squared 522 prediction error (Eq. 9) is close to one. Recall from section 2.4.3 that this statistic 523 measures how well the prediction distribution of the E-BLUP characterizes its un-524 certainty. The mean standardized squared prediction error should be close to one, 525 this is effectively a check on the model-fitting procedure. More sensitive as a test of 526 the fitted LMM are the median values, expected to be close to 0.455 for normally-527 distributed prediction errors. In all cases the values fall within the 95% confidence interval for the sample median with a sample of his size, [0.22, 0.64], suggesting that
the model is reliable. In both cases, the median values are somewhat closer to the
expected value for the model with both covariates included. One possible reason for
this is that the covariates account for outlying values in the data, either marginal
outliers (particularly large or small values) or spatial outliers (values that appear
unusual in spatial context).

Tables 4a and 4b show the results from computing probabilities for each EUNIS 535 sediment class from the cross-validation distributions. The first part of each table 536 shows the comparison between the most-probable class and the observed class, and 537 the associated representations and purities. The overall proportion of validation sites 538 where the most probable class, inferred from the E-BLUP distribution corresponds to 539 the observed class is 0.58 when the only fixed effect is a constant, and is increased to 540 0.65 by inclusion of bathymetry and backscatter as fixed effects. These proportions 541 may be compared with 0.47 (the proportion of sites in the most common class) and 542 0.31 (the probability of correctly allocating the class by guesswork; Eq.11). Note 543 that all class purities are improved by including bathymetry and backscatter (apart 544 from class 'Mixed' which is unaffected) and the representation of all classes apart 545 from Sand and Muddy Sand is also improved. The overall class entropy is 1.27 nats. This is reduced to 1.13 by using the E-BLUP with no covariates, and to 0.96 by the 547 inclusion of bathymetry and backscatter as covariates. 548

#### 549 3.3 Mapping

Figure 8 shows the class of maximum probability according to the E-BLUP with (8a) the constant the only fixed effect and (8b) bathymetry and backscatter included as fixed effects. Given the relatively sparse sampling it is not surprising that the map based only on the sample data is more generalized than the map incorporating the backscatter and bathymetry. In particular, the Mixed class is more restricted in its distribution across the area. Both maps reveal the effect of broad-scale bathymetry (Fig. 2) on the distribution of seabed sediment. Coarser

sediment fractions (including 'coarse' and 'mixed') are typically associated with the
bathymetric platforms within the area, and the bathymetric deep in the southeast of
the study area shows a clear association with mud at seabed. These broad patterns
can be seen in the map in Fig. 8a, which is based on the LMM where the only fixed
effect is a constant and bathymetry is not used for prediction. They are, of course,
more apparent in the map in Fig. 8b, based on the LMM which incorporates the
acoustic data.

Sediment class predictions based on the acoustic data also suggest clearer affini-564 ties between smaller-scale seabed geomorphology and sediment distribution (Fig. 565 8b). This result is consistent with our understanding of the geology of the region 566 e.g., glacially streamlined landforms (NW-SE oriented) are more likely to comprise 567 coarse sediments (e.g., Colgan et al., 2005). This level of detail is not captured by 568 the map presented in Fig. 8a where the acoustic data are not fixed effects in the 569 LMM. Fig. 8c shows some of the predictions from the model with acoustic data 570 at larger scale. This shows the coarser texture of sediment on glacially streamlined 571 landforms (NW-SE orientation) captured by the model prediction where the features 572 are sufficiently large (e.g., between 'Mixed' vs. 'Sand' classes). Note that there are 573 significant variations of landform in Fig. 8c within the area where 'Mud' is the most probable class. 575

Figure 9 shows the probability of the most probable class. Again, the spatial 576 pattern is more general in Fig. 9a with no covariates, and the distribution of sample points dominates the pattern. Note, in both maps, the areas with greater uncertainty 578 in two large areas where 'Coarse' is the most probable class and one in the west of 579 the region where Mud and Sandy Mud is most probable. Not surprisingly, there 580 is greater uncertainty at or near the boundaries between adjacent sediment classes. 581 The vertical striping in Fig. (9b) reveals the persistence of artefacts in the acoustic 582 data through to the modelled outputs. Here the striping artefact mimics the survey 583 track lines, where the outer beams of the acoustic backscatter data are not entirely normalized with those from adjacent lines. This emphasizes the requirement for high quality data acquisition and processing protocols when employing these methods.

As discussed previously, the information in the local prediction distribution of the transformed compositional variables can be presented in terms of the most probable class, and its probability (as in Figs. 8 and 9) but it is also possible to show the probability of occurrence of particular sediment texture classes. For example, Fig. 10 shows the probability of occurrence of texture class 'Coarse'. The two maps show broadly similar spatial patterns, with finer spatial resolution where the acoustic covariates are included.

As discussed in section 2.4.3., the degree of uncertainty in any local prediction distribution, with respect to the probability of the sediment texture classes, is summarized by the classification entropy which is large when the probabilities of each of the set of classes are similar (so uncertainty is greatest). Over 80% of the region the entropy is smaller when the covariates are used (Fig. 11), i.e., the uncertainty about the classes is reduced by incorporating the acoustic information.

#### 600 4. Discussion and Conclusions

Our results show that the predictive accuracy of geostatistical mapping of sedi-601 ment texture classes can be improved by incorporation of bathymetry and backscat-602 ter data. This can be achieved by treating these variables as covariates in the LMM. 603 The prediction is improved as judged from the cross validation error matrices and 604 associated summary statistics, and also by the prediction entropy which shows that 605 the uncertainty is, on average, reduced by the additional information. In contrast 606 to the predictions from the model with a constant mean as the only fixed effect, 607 model predictions incorporating the acoustic data captured finer detail in the distri-608 bution of sediments. These patterns are geologically plausible, reflecting the effects 609 of several environmental processes which act upon the seabed at varying spatial and temporal scales (e.g., sedimentation of finer sediments in lower energy deeps; seabed 611 exposure of coarser sediment associated with glacial landforms). 612

We have demonstrated the value of the LMM and E-BLUP for predicting sed-613 iment texture properties from grab samples and bathymetry and backscatter data 614 in one study area. Further studies are needed to evaluate the method over a wider 615 range of conditions. It is known from previous studies, cited above, that sediment 616 properties are correlated with bathymetry and acoustic backscatter. Furthermore, 617 since sediment properties depend on processes that operate at different spatial scales 618 it is very likely that they will generally show spatial dependence. Given these two 619 considerations it is reasonable to expect that the LMM will be found to be a generally 620 useful model for this purpose. 621

This approach retains the advantages of the ordinary cokriging approach pre-622 sented by Lark et al. (2012), whilst allowing the additional information in the 623 covariates to be exploited. The advantages are that the linear mixed modelling is 624 a robust and reproducible process, with internal model validation (through cross-625 validation on the prediction distributions). It is an objective process, not requiring 626 expert interpretation, which may make it rather more rapid and less costly than con-627 ventional geological mapping. Finally, unlike data mining methods (such as machine 628 learning), the LMM is a formal statistical model. The prediction distributions that 629 are produced from it allow probabilistic assessments to be made of the uncertain 630 allocations of locations to sediment classes, and can also be interrogated directly 631 to provide estimates of the actual sand, mud and gravel content where this is re-632 quired. The covariates, being more densely sampled than the direct observations of sediment, allow more accurate predictions to be made at sites across the study area. 634 Conventional geological mapping of sediments is laborious and requires experi-635

enced staff. However, process-based interpretation of observations provides a sound basis for mapping. In circumstances where an existing sediment map has been produced by geological interpretation, and new data become available (e.g., sediment data and bathymetry and backscatter), then the LMM could be used to update the map by incorporating its units as a fixed effect. In this case the different mapped units become (categorical) fixed effects in the LMM, along with the continuous covariates (bathymetry and backscatter).

While, as noted above, the LMM is a formal probabilistic model unlike data 643 mining methods, the latter can be particularly useful for dealing with non-linear 644 relationships between target variables and predictors. It would therefore be useful 645 to compare the LMM with data mining methods, and expert interpretation, in a 646 range of settings. Such comparative studies have been rare to date, but the one 647 by Diesing et al. (2014) demonstrates their potential value. It would be useful to carry out such studies in a range of conditions to compare the LMM with expert 649 interpretation and data mining methods with respect to both statistical measures of 650 prediction quality and the time and cost requirements of the methods. 651

It was notable that incorporating the covariates into the predictive models had 652 the largest effect on the spatially correlated residual variance; i.e., the covariates 653 largely explained the broader-scale patterns of variation in sediment composition. 654 In the models with covariates included the nugget variance, i.e., the variance not 655 resolved by sampling, was larger than the correlated variance. The fine-scale varia-656 tion in the ALR-mud and ALR-sand were strongly correlated, suggesting that they 657 reflect common processes that these covariates did not capture. As a result, the 658 final map gives a good impression of the general trends in sediment composition, 659 but predicted variations over short distances are less certain. 660

The structure of the LMM lends itself to the incorporation of additional information. For example, geomorphological interpretation of bathymetry, or continuous predictors based on the bathymetric surface (rugosity, slope etc.) might be incorporated as covariates. Hydrodynamic model outputs (e.g., current speeds and wave orbital velocity) might similarly be incorporated as predictors, and the log-ratio testing procedure used here can be applied to evaluate the evidence for particular sources of information before a particular model is used for prediction. Finally, one possible way to reduce the residual variance of the model at the finest scales might be

through physical modelling of the characteristics of the backscatter (e.g., Sternlicht and de Moustier, 2003).

In conclusion, the LMM was shown to be an effective method to incorporate 671 backscatter and bathymetry information into the prediction of sediment texture 672 classes. There is scope to use this approach to incorporate a wider range of pre-673 dictors, including outputs from physical models or other variables derived from 674 bathymetry. It could also be used to incorporate conventional geological maps of 675 the seabed as a way to update these with new data. There is scope for further work 676 to develop this method (particularly for upscaling predictions) and to compare it 677 with other approaches. 678

# 679 Acknowledgements

The contributions of RML, BPM, DD, SLG and HS are published with the permission of the Executive Director of the British Geological Survey (NERC), and this work was supported by NERC's Marine Environmental Mapping (MAREMAP) programme (http://www.maremap.ac.uk). Multibeam echosounder and grab sampling data were collected as part of the 'Coordination of the Defra Marine Conservation Zone data collection programme 2011/12' funded by the Department of Environment, Food and Rural Affairs of the United Kingdom.

#### References

- Aitchison, J., 1986. The Statistical Analysis of Compositional Data. Chapman and Hall, London.
- Akaike, H., 1973. Information theory and an extension of the maximum likelihood principle. In: Petov, B.N., Csaki, F. (Eds.), Second International Symposium on Information Theory. Akademia Kiado, Budapest, pp. 267–281.
- Anderson, J.T., Gregory, R.S., Collins, W.T., 2002. Acoustic classification of marine habitats in Newfoundland. ICES Journal of Marine Science 59, 156–167.
- Bale, A.J., Kenny, A.J., 2005. Sediment analysis and seabed characterization. In: N.A. Holme, N.A., McIntyre, A.D. (Eds.), Methods for the study of marine benthos. Blackwell, Oxford, pp. 43–86.
- Brown, C.J., Smith, S.J., Lawton, P., Anderson, J.A.T., 2011. Benthic habitat mapping: A review of progress towards improved understanding of the spatial ecology of the seafloor using acoustic techniques. Estuarine, Coastal and Shelf Science 92, 502–520.
- Burgess, T.M., Webster, R., 1980. Optimal interpolation and isarithmic mapping of soil properties. II Block kriging. Journal of Soil Science 31, 333–341.
- Clark, C.D., Hughes, A.L.C., Greenwood, S.L., Jordan, C.J., Sejrup, H.P., 2012.
  Pattern and timing of retreat of the last British-Irish Ice Sheet. Quaternary
  Science Reviews 44, 112–146.
- Colgan, P.M., Kickelson, D.M., Cutler, P.M., 2005. Ice-marginal terrestrial landsystems: southern Laurentide ice sheet margin. In: Evans, D.J.A. (Ed.), Glacial Landsystems. Hodder Arnold, London, pp. 111–142.
- Connor, D.W., Gilliland, P.M., Golding, N., Robinson, P., Todd, D., Verling, E., 2006. UKSeaMap: the mapping of seabed and water column features of UK Seas. Joint Nature Conservation Committee, Peterborough.

- Dartnell, P., Gardner, J.V., 2004. Predicting seafloor facies from multibeam bathymetry and backscatter data. Photogrammetric Engineering and Remote Sensing 70, 1081–1091.
- Diesing, M., Green, S.L., Stephens, D., Lark, R.M., Stewart, H.A., Dove, D., 2014.
  Mapping seabed sediments: Comparison of manual, geostatistical, object-based image analysis and machine learning approaches. Continental Shelf Research 84, 107–119.
- Endler, M., Endler, R., Bobertz, B., Leipe, T., Arz, H.W., 2015. Linkage between acoustic parameters and seabed sediment properties in the south-western Baltic Sea. Geo-Marine Letters 35, 145–160.
- Evans, J.L., Peckett, F., Howell, K.L., 2015. Combined application of biophysical habitat mapping and systematic conservation planning to assess efficiency of representativeness of the existing High Seas MPA network in the Northeast Atlantic. ICES Journal of Marine Science 72, 1483–1497.
- Everest, J., Bradwell, T., Golledge, N., 2005. Subglacial landforms of the Tweed palaeo-ice stream. The Scottish Geographical Magazine 121, 163–173.
- Folk, R.L., 1954. The distinction between grain size and mineral composition in sedimentary rock nomenclature. Journal of Geology 62, 344–359.
- Fonseca, L., Brown, C., Calder, B., Mayer, L., Rzhanov, Y., 2009. Angular range analysis of acoustic themes from Stanton Banks Ireland: A link between visual interpretation and multibeam echosounder angular signatures. Applied Acoustics 70, 1298–1304.
- Gatliff, R. W., Richards, P.C., Smith, K., Graham, C.C., McCormac, M., Smith, N. J. P., Long D., Cameron, T.D.J., Evans, D., Stevenson, A.G., Bulat, J., Ritchie, J.D., 1994. United Kingdom offshore regional report: the geology of the central North Sea. British Geological Survey, HMSO, London.

- Glynn, B., Brown, C., Rooney, S., 2008. Coincident swath acoustic backscatter and bathymetry for the interpretation of shallow-water sediment composition and processes. Journal of the Geological Society 165, 597–607.
- Goff, J.A., Kraft, B.J., Mayer, L.A., Schock, S.G., Sommerfield, C.K., Olson, H.C., Gulick, S.P.S., Nordfjord, S., 2004. Seabed characterization on the New Jersey middle and outer shelf: correlatability and spatial variability of seafloor sediment properties. Marine Geology 209, 47–172.
- Graham, A.G.C., Stoker, M.S., Lonergan, L., Bradwell, T., Stewart, M.A., 2011.

  The Pleistocene glaciations of the North Sea basin. Developments in Quaternary Science 15, 261–278.
- Haris, K., Chakraborty, B., 2014. Stochastic formalism-based seafloor feature discrimination using multifractality of time-dependent acoustic backscatter. Nonlinear Processes in Geophysics 21, 101–113.
- Howell, K.L., 2010. A benthic classification system to aid in the implementation of marine protected areas networks in the deep/high seas of the NE Atlantic. Biological Conservation 143, 1041–1056.
- Hughes Clarke, J.E., Mayer, L.A., Wells, D.E., 1996. Shallow-water imaging multibeam sonars: a new tool for investigating seafloor processes in the coastal zone and on the continental shelf. Marine Geophysical Researches 18, 607–629.
- Huntley, D.A., Huthnance, J.M., Collins, M.B., Liu, C-L., Nicholls, R.J., Hewitson, C., Green, M.O., Dyer, K.R., Jago, C.F., 1993. Hydrodynamics and sediment dynamics of North Sea sand waves and sand banks. Philosophical Transactions of the Royal Society of London. Series A: Physical and Engineering Sciences 343, 461–474.
- International Association of Oil & Gas Producers, 2013. Guidelines for the conduct of offshore drilling hazard site surveys. International Association of Oil & Gas

- Producers Report No. 373-18-1 http://www.ogp.org.uk/pubs/373-18-1.pdf
- International Hydrographic Organization, 2008. IHO standards for hydrographic surveys, 5<sup>th</sup> Edition, IHO Special Publication S-44, International Hydrographic Bureau, Monaco.
- Journel, A.G., Huijbregts, C.J., 1978. Mining Geostatistics. Academic Press, London.
- 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. Marine Ecology Progress Series, 219, 121–137.
- Lark, R.M., 1995. Components of accuracy of maps with special reference to discriminant analysis on remote sensor data. International Journal of Remote Sensing 16, 1461–1480.
- Lark, R.M., Dove, D., Green, S.L., Stevenson, A., Stewart, H., Stevenson, A., 2012. Spatial prediction of seabed sediment texture classes by cokriging from a legacy database of point observations. Sedimentary Geology 281, 35–49.
- Long, D., 2006. BGS detailed explanation of seabed sediment modified Folk classification. MESH (Mapping European Seabed Habitats) available at <a href="http://www.searchmesh.net/PDF/GMHM\_Detailed\_explanation\_of\_seabed\_sediment\_classification.pd">http://www.searchmesh.net/PDF/GMHM\_Detailed\_explanation\_of\_seabed\_sediment\_classification.pd</a>
- Lucieer, V., Hill, N.A., Barrett, N.S., Nichol, S., 2013. Do marine substrates 'look' and 'sound' the same? Supervised classification of multibeam acoustic data using autonomous underwater vehicle images. Estuarine, Coastal and Shelf Science 117, 94–106.
- Marchant, B.P., Lark, R.M., 2007. Estimating of linear models of coregionalization by residual maximum likelihood. European Journal of Soil Science 58, 1506–1513.

- Marsh, I., Brown, C., 2009. Neural network classification of multibeam backscatter and banthymetry data from Stanton Bank (Area IV). Applied Acoustics 70, 1269–1276.
- Martín-Fernandéz, J.A., Thió-Henestrosa, S., 2006. Rounded zeros: some practical aspects for compositional data. In: Buccianti, A., Mateu-Figueras, G., Pawlowsky-Glahn, V. (Eds.), Compositional Data Analysis in the Geosciences: From Theory to Practice. Geological Society of London Special Publications 264, pp. 191–201.
- McGonigle, C., Collier, J., 2014. Interlinking backscatter, grain size and benthic community structure. Estuarine, Coastal and Shelf Science 147, 123–136.
- Patterson, H.D., Thompson, R., 1971. Recovery of inter-block information when block sizes are unequal. Biometrika 58, 545–554.
- Pawlowsky-Glahn, V., Olea, R.A., 2004. Geostatistical Analysis of Compositional Data. Oxford University Press, New York.
- Snellen, M., Siemes, K., Simons, D., 2011. Model-based sediment classification using single-beam echosounder signal. Journal of the Acoustic Society of America 129, 2878–2888.
- Stein, M.L., 1999. Interpolation of spatial data: some theory for kriging. Springer, New York.
- Sternlicht, D.D., de Moustier, C.P., 2003. Time dependent seafloor acoustic backscatter (10–100 kHz). Journal of the Acoustic Society of America 114, 2727–2743.
- Stokes, C.R., Clark, C.D., 2001. Palaeo-ice streams. Quaternary Science Reviews 20, 1437–1457.
- Stokes, C.R., Spagnolo, M., Clark, C.D., 2011. The composition and internal structure of drumlins: Complexity, commonality, and implications for a unifying theory of their formation. Earth-Science Reviews 107, 398–422.

- Verbeke, G., Molenberghs, G., 2000. Linear Mixed Models for Longitudinal Data. Springer-Verlag, New York.
- Wentworth, C.K., 1922. A scale of grade and class terms for clastic sediments. The Journal of Geology 30, 377–392.

 ${\bf Table\ 1}\ {\bf Summary\ statistics\ of\ particle\ size\ class\ data}.$ 

	Sand Per	Mud cent by	0.10.101
	1 01		111000
Mean	72.93	14.22	12.85
Median	75.23	13.66	9.43
Standard deviation	12.91	7.86	12.97
First quartile	64.02	8.3	1.07
Third quartile	79.36	20.84	21.68
Minimum	42.58	1.13	0.00
Maximum	98.76	31.9	45.11
Minimum non-zero	42.58	1.13	0.018
value			

**Table 2** Results for model-fitting.

		*	٠
	$\lambda^{ m M}$	0.402	0.095
	$\lambda^{\mathrm{S}}$	0.791	0.767
	$c_1^{ m S,M}$	0.362 0.791	0.006
*%	$\phi  c_0^{\mathrm{S,S}}  c_0^{\mathrm{M,M}}  c_0^{\mathrm{S,M}}  c_1^{\mathrm{S,S}}  c_1^{\mathrm{M,M}}  c_1^{\mathrm{S,M}}  \lambda^{\mathrm{S}}  \lambda^{\mathrm{M}}$	0.551  12495  0.482  0.041  0.138  0.857  0.164	8911 0.395 0.013 0.069 0.011 0.007 0.006 0.767
rameter	$c_1^{ m S,S}$	0.857	0.011
Variance parameters*	$c_0^{ m S,M}$	0.138	0.069
	$c_0^{ m M,M}$	0.041	0.013
	$c_0^{\mathrm{S,S}}$	0.482	0.395
	φ	12495	8911
	$\mathcal{A}$	0.551	0.658
AIC		-80.2 $-111.6$ $-120.6$	-129.8 0.658
P		42.1 59.8 64.3	70.9
$N_p$		0.44	9
Fixed effects		Constant only Constant + bathymetry Constant + backscatter	Constant + bathymetry + backscatter

Parameters include the Box-Cox transform parameter,  $\lambda^{S}$  and  $\lambda^{M}$  for ALR-Sand or ALR-Mud respectively. ALR data were first scaled to unit variance and then a constant was added to ensure all positive values.

 ${\bf Table~3~Cross\text{-}validation~results~for~(Box\text{-}Cox~transformed)~ALR\text{-}Sand~and~ALR\text{-}} \\ {\bf Mud.}$ 

Fixed effects	Mean square error			Standardized square prediction error		
	Sand	Mud	Me Sand	ean Mud	Med Sand	dian Mud
Constant only	0.76	0.09	1.03	1.04	0.38	0.33
Constant + acoustic bathymetry + acoustic backscatter	0.44	0.02	1.05	1.05	0.46	0.35

**Table 4a** Cross-validation results for prediction of sediment texture classes; constant the only fixed effect.

Distribution of observations					
	Most probable class				-
Observed	Coarse	Mixed	Mud &	Sand &	
Class			Sandy Mud	Muddy Sand	Representation
Coarse	8	0	1	3	0.66
Mixed	4	22	3	7	0.61
Mud &					
Sandy Mud Sand &	1	4	8	3	0.50
Muddy Sand	3	3	0	7	0.54
Purity	0.50	0.76	0.66	0.35	

Proportion of validation sites	
in most-probable class	0.58
Expected proportion correct	
by random allocation	0.31
•	
Proportion in commonest class	
(Mixed)	0.47
Cl	1.07
Class entropy	1.27
Mean prediction entropy	1.13
T T T T T T T T T T T T T T T T T T T	

**Table 4b** Cross-validation results for prediction of sediment texture classes; acoustic bathymetry and backscatter as fixed effects.

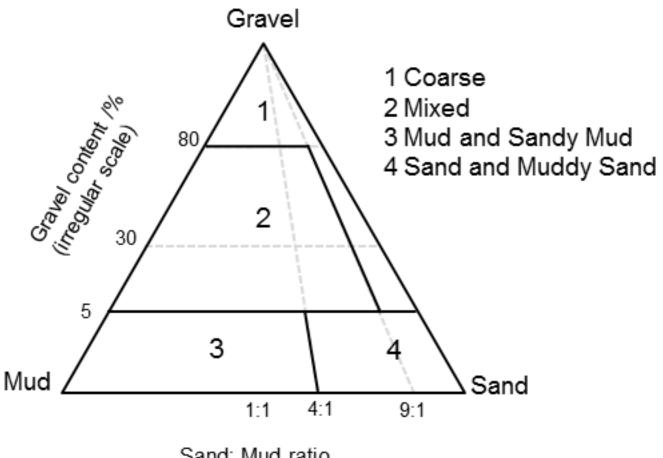
Distribution of observations						
	Most probable class					
Observed	Coarse	Mixed	Mud &	Sand &		
Class			Sandy Mud	Muddy Sand	Representation	
Coarse	9	2	0	1	0.75	
Mixed	5	25	$\frac{\circ}{2}$	4	0.69	
$\mathrm{Mud}\ \&$						
Sandy Mud	0	1	10	5	0.63	
Sand &		_			0.40	
Muddy Sand	2	5	0	6	0.46	
Purity	0.56	0.76	0.83	0.38		

Proportion of validation sites	0.65
in most-probable class	0.00
Expected proportion correct by random allocation	0.31
Proportion in commonest class (Mixed)	0.47
Class entropy	1.27
Mean prediction entropy	0.96

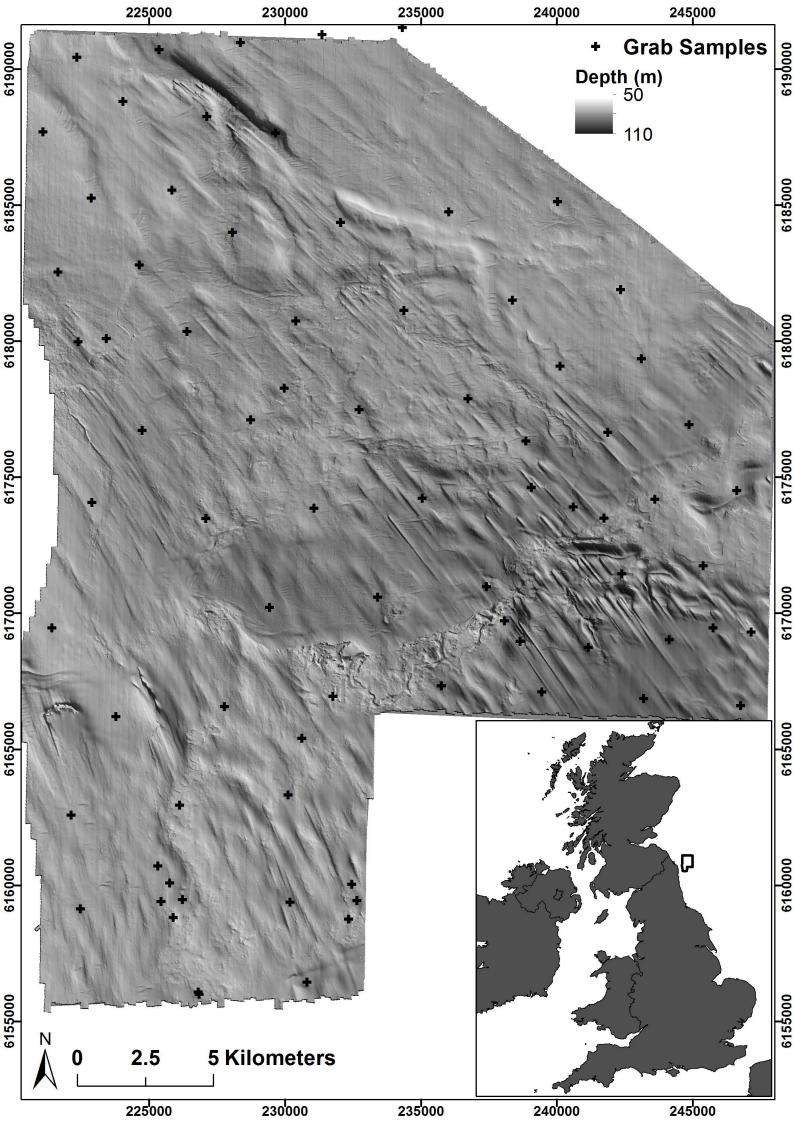
## Figure Captions

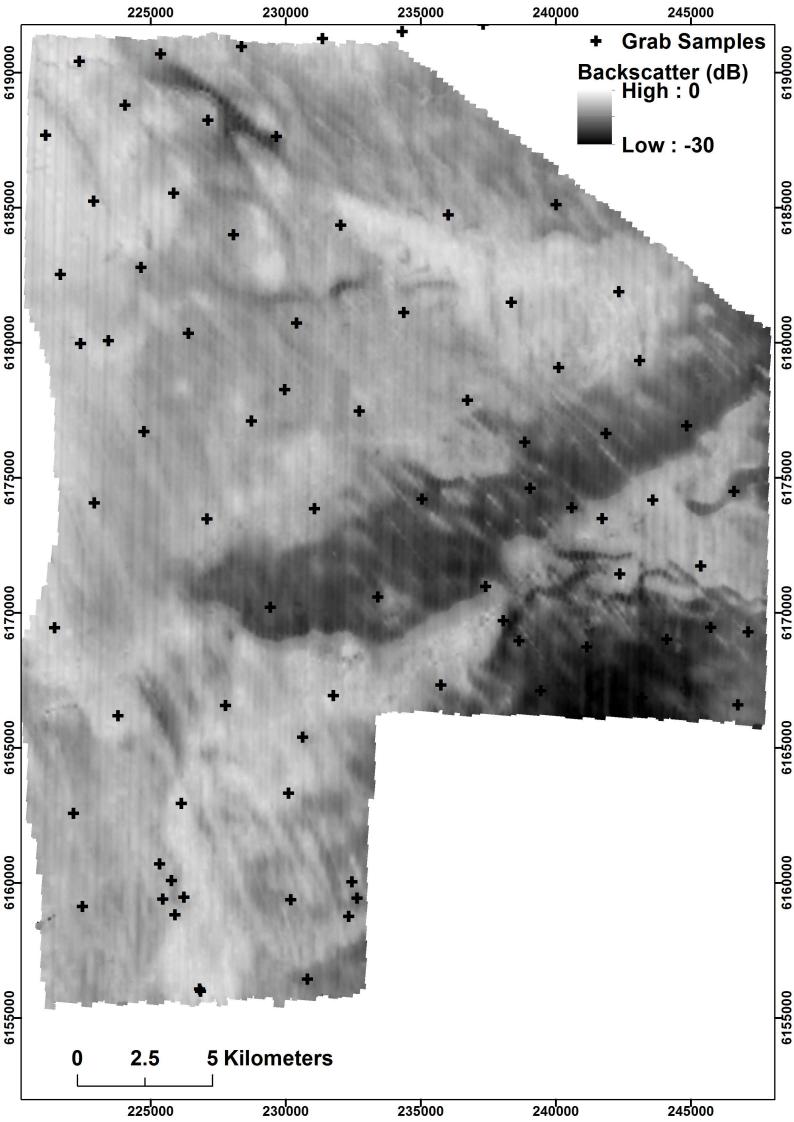
- **Figure 1**. EUNIS sediment texture classes defined on the ternary diagram for silt, mud and sand.
- Figure 2. High-resolution swath bathymetry of the study area with grab sample locations indicated. The location of the study area off the northeast coast of England is shown in inset. Acoustic and ground-truthing data provided courtesy of Defra.
- **Figure 3**. Acoustic backscatter data expressed in decibels (dB) with grab sample locations indicated. Acoustic and ground-truthing data provided courtesy of Defra.
- **Figure 4.** Post-plot of ALR-transformed sand and mud content. The data are divided into four sets defined by the quartiles of the distribution, so 'Q1' indicates observations smaller than the first quartile, i.e., the smallest 25% of all data.
- **Figure 5**. Histograms of ALR-transformed sand and mud content (top), scatter plots of ALR-transformed sand and mud content and acoustic bathymetry and backscatter with correlation coefficients (R) (bottom).
- **Figure 6.** Scatterplots of ALR-transformed sand and mud content against acoustic backscatter (top) and bathymetry (bottom). Correlation coefficients (R) are also shown.
- Figure 7. Histograms of cross-validation kriging errors for Box-Cox transformed values of ALR-Sand and ALR-Mud using model with constant mean the only fixed effect (top) or the selected model with both acoustic bathymetry and backscatter as fixed effects (bottom).
- **Figure 8**. Class of maximum probability according to E-BLUP distribution with (a) constant only fixed effect, (b) bathymetry and backscatter as fixed effects,

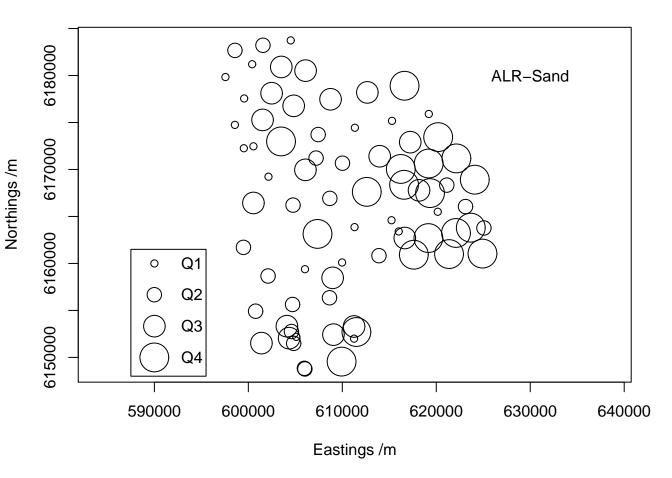
- (c) a section of the map obtained using bathymetry and backscatter in shown at larger scale. The rectangle on (b) indicates the area of (c). Sediment class predictions are overlain on shaded-relief backscatter.
- **Figure 9**. Probability of class of maximum probability according to E-BLUP distribution with (a) constant only fixed effect, and (b) bathymetry and backscatter as fixed effects.
- Figure 10. Probability of class 'Coarse' according to E-BLUP distribution with (a) constant only fixed effect, and (b) bathymetry and backscatter as fixed effects.
  Values are overlain on shaded-relief bathymetry to demonstrate association between geomorphology and seabed sediment distribution.
- **Figure 11**. Entropy of class prediction probabilities according to E-BLUP distribution with (a) constant only fixed effect and (b) bathymetry and backscatter as fixed effects.

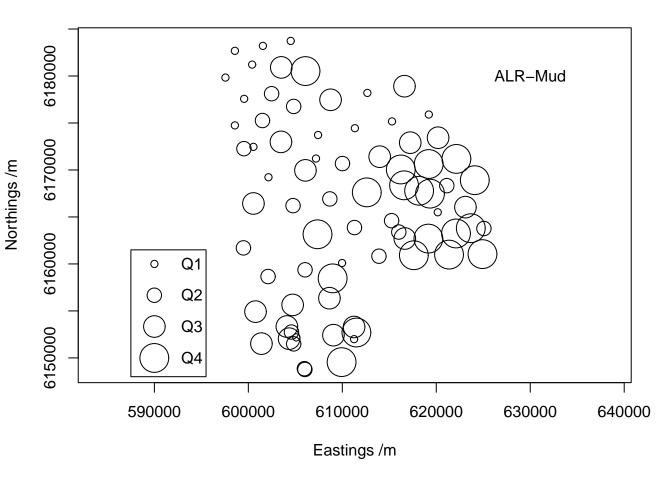


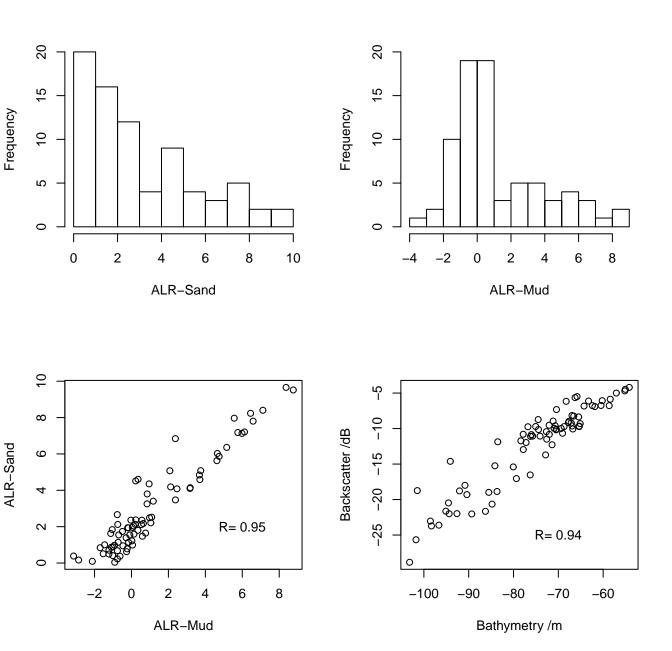
Sand: Mud ratio (irregular scale)

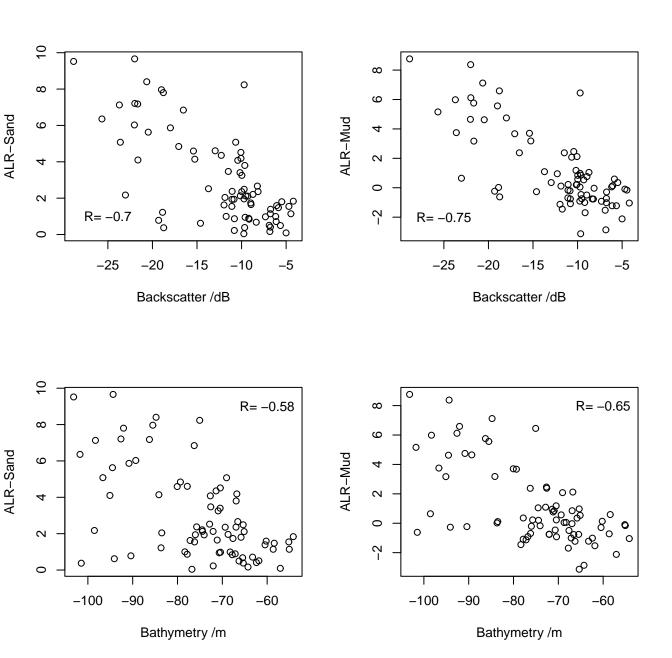


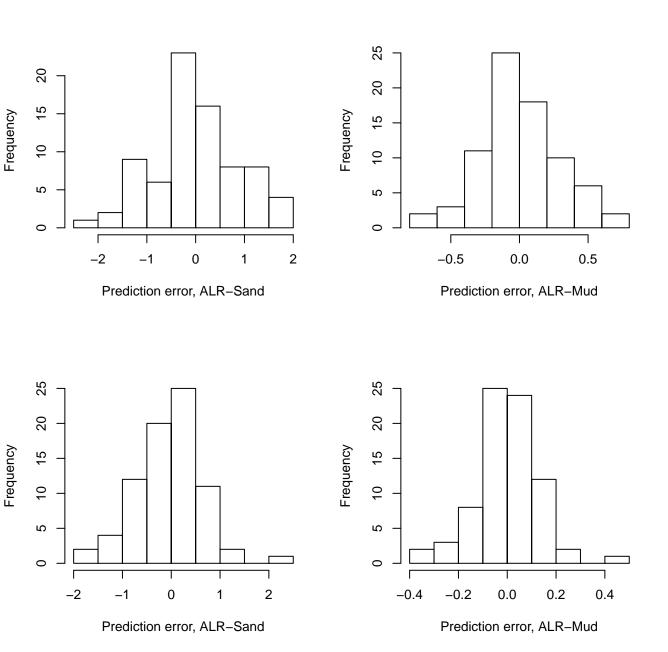


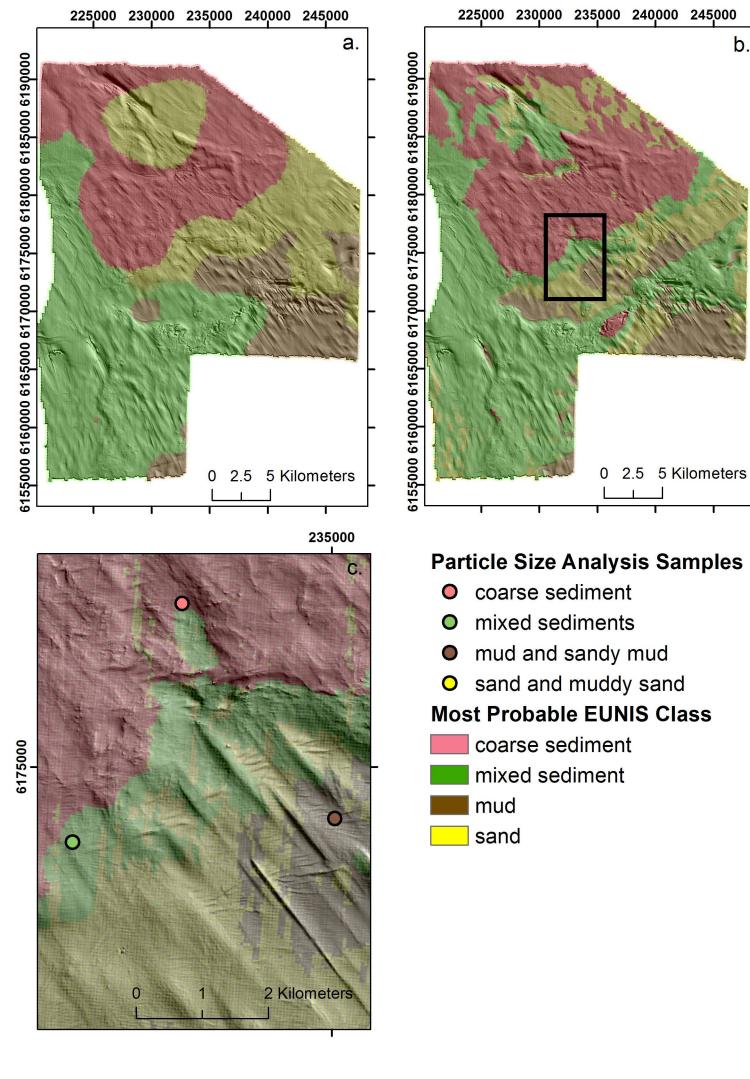












b.

