1 Predictive mapping of organic carbon stocks and accumulation rates

2 in surficial sediments of the Canadian continental margin

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16 Abstract

The quantification and mapping of surficial seabed sediment organic carbon has wide-scale 17 18 relevance across marine ecology, geology and environmental resource management, with carbon densities and accumulation rates being a major indicator of geological history, ecological function, 19 20 and ecosystem service provisioning, including the potential to contribute to nature-based climate 21 change mitigation. While global mapping products analyses can appear to provide a definitive understanding of the spatial distribution of sediment carbon, there is inherently high uncertainty 22 23 when making estimates at this scale. Finer resolution national regional maps may be constructed 24 at finer resolutions and can which utilise targeted data syntheses and refined spatial data products 25 are and therefore vital to have the potential to improve these estimates. Here, we report a national 26 systematic review of data on organic carbon content in seabed sediments across Canada and 27 combine this with a synthesis and unification of best available data on sediment composition, 28 seafloor morphology, hydrology, chemistry, and geographic settings and sediment mass 29 accumulation rates within a machine learning mapping framework. Predictive quantitative maps 30 of mud content, sediment dry bulk density, and organic carbon content and, organic carbon 31 density and accumulation, were each produced along with cell specific estimates of their 95% confidence interval (CI) bounds uncertainty at 200 m resolution across 4,489,235 km² of the 32 Canadian continental margin (92.6% of the seafloor area above 2,500 m). Fine-scale variation in 33 carbon stocks was identified across the Canadian continental margin, particularly in the Pacific 34 and Atlantic Ocean regions. Carbon accumulation was predicted to be concentrated in coastal 35 areas, with the highest rates in the Gulf of St Lawrence and Bay of Fundy. Overall, we estimate 36 the standing stock of organic carbon in the top 30 cm of surficial seabed sediments across the 37 Canadian shelf and slope to be 10.7-9 Gt (95% CI-67.60 - 16.0 Gt), and accumulation at 4.9 Mt 38 per year (95% Cl 2.6 - 9.3 Mt y⁻¹). Increased *in-situ* empirical sediment data collection and higher 39 40 precision in spatial environmental data-layers could significantly reduce uncertainty and increase 41 accuracy in these products over time.

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43 **1. Introduction**

The organic carbon contained in seafloor sediments has a major influence on global carbon cycles and earth's climate (Hülse et al., 2017; Bauer et al., 2013). Seabed sediments have been estimated to accumulate approximately 126–350 Mt of organic carbon per year (Keil, 2017; Berner, 1982) and contain 87 Gt of organic carbon in their top 5 cm (Lee et al., 2019), 168 Gt in 48 the top 10 cm (LaRowe et al., 2020a) and up to \sim 2,300 Gt in the top 1 m (Atwood et al., 2020), 49 with the latter being equivalent to nearly twice that of soils on land. Continental shelves have the 50 highest concentrations densities of sediment carbon across the global ocean, covering only 5-8% of the marine area but an estimated 15-19% of surficial organic carbon stocks (LaRowe et al., 51 2020a; Atwood et al., 2020) and 80% of annual carbon burial (Bauer et al., 2013; Burdige, 2007). 52 Continental margin zones (continental shelves and slopes) also contain the largest spatial 53 54 variation in organic carbon densities due to highly heterogenous geological, geographic, biological and oceanographic settings (Smeaton et al., 2021; Diesing et al., 2017, 2021; Atwood et al., 55 56 2020). They are also subjected to high levels of human activity, being impacted by many coastal 57 and marine industries including fishing, shipping, energy generation, telecommunication, mineral extraction, and pollution from land based activities- (Halpern et al., 2019; Amoroso et al., 2018; 58 59 Keil, 2017). The quantification and mapping of organic carbon on continental margins is therefore imperative for best practise seabed management; with the densities and accumulation rates being 60 61 a major indicator of ecological function, geological history and ecosystem service provision (Legge et al., 2020; Snelgrove et al., 2018; Middelburg, 2018). 62

63 In the marine environment, organic carbon can originate from the fixation of carbon dioxide (CO_2) 64 by primary producers in the photic zone or via lateral transport from terrestrial sources (LaRowe et al., 2020b). Organic carbon then passes through a variety of biotic and abiotic pathways being 65 66 consumed, transformed, respired or remineralised, with a large proportion converted back into inorganic compounds, leaving only ~5% of marine production and less than 1% of earth's gross 67 production eventually reaching the seafloor (Middelburg, 2019; Hülse et al., 2017; Turner, 2015; 68 Bauer et al., 2013; Burdige, 2007). Once at the seafloor, a similarly complex process occurs on 69 and within the sediment, with a wide range of biotic, biochemical and physical processes all 70 71 influencing the rates of accumulation, remineralisation and resultant long term burial, with ~90% 72 of all carbon reaching the seafloor being remineralised (LaRowe et al., 2020b; Middelburg, 2018, 73 2019; Arndt et al., 2013). Even when considering this complex carbon cycle, the mass and accumulation of organic carbon in surficial seabed sediments will still have a direct influence on 74 75 the scale of long-term carbon storage at the seafloor (LaRowe et al., 2020a; Middelburg, 2018).

Marine habitats are being increasingly recognised as contributors to nature-based climate change mitigation (also known as nature-based climate solutions and natural climate solutions) due to their ability to both fix CO₂ and store organic carbon for centennial to millennial timescales (Macreadie et al., 2021; Hoegh-Guldberg et al., 2019). This "blue carbon" potential was initially recognised in coastal vegetated habitats (i.e. mangrove, seagrass and saltmarsh) (Nellemann et 81 al., 2009; Duarte et al., 2005), but has more recently been applied to other habitats such as kelp 82 forests and unvegetated sediments (Luisetti et al., 2020; Raven, 2018; Avelar et al., 2017). There 83 is increasing evidence that human activities are influencing seabed sediment carbon stores from both perturbations of upstream processes and physical impacts directly on the seafloor (Cavan 84 and Hill, 2022; Epstein et al., 2022; Keil, 2017; Bauer et al., 2013). For example, a recent study 85 estimated that the direct physical impacts from global fishing activities could cause considerable 86 87 remineralisation of seabed sediment organic carbon stocks back to CO₂ (Sala et al., 2021), 88 however the validity of the scale of these estimates has been called into question (Hiddink et al., 2023; Hilborn and Kaiser, 2022; Epstein et al., 2022). By improving the accuracy in available 89 90 sediment carbon mapping products, there may be potential opportunities to better research and design appropriate management strategies to enhance organic carbon accumulation or limit 91 potential remineralisation from disturbance (Epstein and Roberts, 2022; Sala et al., 2021; Luisetti 92 et al., 2019). 93

94 Historically, studies measuring seabed sediment carbon stocks and accumulation rates had small 95 geographic scope, largely considering the ecological function, geological characteristics or 96 biochemical functioning at local to regional scales (see citations within LaRowe et al., 2020b; 97 Snelgrove et al., 2018; Middelburg, 2018; Burdige, 2007). In recent years, made possible by modern machine learning and statistical spatial prediction techniques, there has been increasing 98 99 interest in estimating the size and distribution of carbon standing stocks and accumulation rates at national to global scales to better understand natural carbon cycles and biological productivity, 100 and to identify the potential for improved management as a natural climate mitigation strategy 101 102 (Restreppo et al., 2021; Smeaton et al., 2021; Diesing et al., 2021; Atwood et al., 2020; LaRowe 103 et al., 2020b; Lee et al., 2019; Wilson et al., 2018; Avelar et al., 2017). Although global mapping 104 products can appear to give a complete understanding of seabed sediment organic carbon stocks 105 , there is high inherent uncertainty when making estimates at this scale (Ludwig et al., 2023; Atwood et al., 2020; Lee et al., 2019), regional mapping studies which utilised targeted data 106 syntheses, refined spatial data products and finer resolution outputs, have shown distinct spatial 107 108 patterns in organic carbon distribution and disparate estimates of total standing stocks when compared with these global studies.- This has been highlighted by several regional studies across 109 110 the northwest European shelf (Smeaton et al., 2021; Diesing et al., 2017, 2021; Luisetti et al., 2020; Wilson et al., 2018). , which show distinct spatial patterns in organic carbon distribution and 111 112 disparate estimates of total standing stocks when compared with these global studies.

113 Canada has the world's longest coastline and approximately the seventh largest Exclusive 114 Economic Zone (EEZ) (Fig. 1), it could therefore be expected to contain a significant proportion 115 of the global stock of seabed sediment organic carbon. Data from recent global studies estimated that the Canadian EEZ contains approximately 2.2 Gt of organic carbon in the top 5 cm and 48 116 Gt in the top meter of seabed sediments, equivalent to ~2.3% of total global marine sediment 117 carbon stocks covering around 1.3% of the area (Atwood et al., 2020; Lee et al., 2019). However, 118 119 these modelled estimates from global studies are at coarse spatial resolutions, have incomplete 120 coverage of the Canadian EEZ and contain very limited *in-situ* empirical data from within the 121 Canadian EEZ itself. The Canadian marine environment is extremely complex, covering three 122 oceans, 46 degrees of latitude, 94 degrees of longitude, and containing numerous features 123 including the largest enclosed marine bay in the world, over 50,000 islands, and on the 124 comparatively short Pacific coastline alone, around 436 estuaries. It is therefore highly likely that 125 global estimates of the distribution of seabed sediment organic carbon stock and accumulation 126 rates are inaccurate for this region, and a national approach is needed. Here, we conduct a systematic review of data on seabed sediment organic carbon content across Canada and 127 128 combine this with a synthesis and unification of best available data on sediment composition, 129 seafloor morphology, hydrology and, chemistry and sediment mass accumulation rates in a 130 machine learning predictive mapping process, to construct the first high-resolution national 131 assessment of Canadian seabed sediment organic carbon stocks and accumulation rates. To aid 132 clarity, a workflow diagram of the proceeding methods and results sections is shown in Figure 2.



- 134 Figure 1. Map of the Canadian Exclusive Economic Zone (EEZ). The study area spatial maxima (red) was defined
- 135 using best available bathymetry data and covers the entire sub-tidal portion of the Canadian EEZ (red; see high
- resolution figure for further detail around the coastline and Section 2.1.1 for more details)-covers the entire sub-tidal
- 137 portion of the Canadian EEZ. This is overlayed by the maximum potential modelling extent (grey) which only includes
- 138 <u>indicates only</u> those areas where data were present for all predictor variables (see Section 2.1.7). Due to the distribution
- of available <u>response</u> data, the final modelling domain was limited to a depth of 2,500 meters (see Section 2.4), and is
- 140 indicated with the colour relative to the estimated depth, from 0 (dark-light blue) to -2,500 (yellowblack). Country outlines
- 141 from World Bank Official Boundaries, available at <u>https://datacatalog.worldbank.org/search/dataset/0038272</u>.

143 2. Methods

144 2.1 Analysis software

Analyses were primarily undertaken in R 4.2.2 (R Core Team. 2022) and RStudio 2022.12.0.353 145 146 (Posit Team, 2022), with some additional data manipulation and spatial plotting in QGIS 147 (QGIS.org, 2021) and Python (Van Rossum and Drake, 2009). Within R, raster data were handled 148 using the terra package (Hijmans, 2022), spatial vector data using the sf package (Pebesma, 149 2018), netCDF data with the stars (Pebesma, 2022) and tidync (Sumner, 2022) packages, dataframes with the dplyr package (Wickham et al., 2019), and vector data with base R (R Core Team, 150 151 2022). Random forest modelling was primarily dependent on the ranger package (Wright and 152 Ziegler, 2017), however models were constructed and tuned using the tidymodels package (Kuhn 153 and Wickham, 2020), with cross-validation and prodictor variable selection using the 154 (Meyer et al., 2023) and caret (Kuhn, 2022) packages. Plotting utilised the above packages as well as ggplot2 (Wickham et al., 2019) and patchwork (Pedersen, 2022) while parallel processing 155 used the doParallel package (Microsoft Corporation and Weston, 2022). To aid clarity, a workflow 156 157 diagram of the proceeding methods and results sections is shown in Figure 2.



Figure 2. Study workflow diagram. Outline of the structure and linkages within the proceeding methods and results
 sections. Light blue shapes indicate input data; white ovals indicate data processes; dark shapes indicate output data;
 rectangles indicate point raster data; circles indicate raster point data. OC = organic carbon; MAR = mass accumulation

164 <u>2. Methods</u>

- 165 2.12 Study area spatial maximaPredictor variables
- 166 <u>2.1.1 Bathymetry</u>

Best available contiguous Digital Elevation Model (DEM) data were combined and unified to a
 200 m x 200 m equal area grid covering the Canadian EEZ (co-ordinate reference system (CRS)
 EPSG:3573 - WGS 84 - North Pole Lambert Azimuthal Equal Area Canada) (Table 1; see
 Appendix A2 for further details). Data were filtered to contain only sub-tidal areas (those cells with
 elevations of less than or equal to 0 m), with the resultant extent defined as the study area spatial
 maxima (Fig. 1).

To define the maximum potential spatial coverage of this study, best available bathymetric 173 174 datasets were combined across the Canadian Exclusive Economic Zone (EEZ) (Table 1). Firstly, three Digital Elevation Model (DEM) raster layers covoring different extents of the Canadian EEZ 175 were each filtered to contain only those elevations of less than or equal to 0 m. Where necessary, 176 177 data were then aggregated (averaged) or disaggregated (split) to a resolution of approximately 178 200 m, and all layers were projected onto a unified 200 m x 200 m equal area grid (co-ordinate reference system (CRS) EPSG:3573 - WGS 84 - North Pole Lambert Azimuthal Equal Area 179 180 Canada). Reprojection was necessary as all three DEMs were in different co-ordinate systems, 181 including some already being projected. The 200 m resolution was chosen as it is the median native resolution of the three DEMs, while also being considered towards the upper limit of what 182 may be computationally possible within the scope of this study. After reprojection, the three layers 183 were overlain, with the region specific data given priority over global data where present. Finally, 184 the seaward boundaries were delineated by the outer extent of the Canadian EEZ (Flanders 185 Marine Institute, 2019). The resultant bathymetric layer was defined as the study area spatial 186 187 maxima and used as the first potential predictor variable in predictive modelling (Fig. 1 - covering 188 all coloured areas; Table 1).

189 **Table 1. Summary of predictor variables constructed for the Canadian EEZ.** For more information on methods

used to derive these layers see Sections 2.1 and 2.2.

Predictor variable	Unit	Region	Source	Native	Temporal	
				resolution	range	
Bathymetry	m	BC	NRCan (2021)	10 m	NA	
		Arctic	IBCAO V4.2 (Jakobsson et al., 2020)	200 m	NA	
		Global	GEBCO (2022)	0.0042°	NA	
Slope	0	Canada	This study	200 m	NA	
Slope smoothed	0	Canada	This study	1 km	NA	
Total curvature	rad/m	Canada	This study	200 m	NA	
Total curvature smoothed	rad/m	Canada	This study	1 km	NA	
BPI – fine	m	Canada	This study	200 m	NA	
BPI medium	m	Canada	This study	400 m	NA	
BPI broad	m	Canada	This study	400 m	NA	
VRM – fine	-	Canada	This study	200 m	NA	
VRM — medium	-	Canada	This study	200 m	NA	
VRM – broad	-	Canada	This study	400 m	NA	
Distance to shore	m	Canada	This study	200 m	NA	
Bioregion	-	Canada	DFO (2022)	NA	NA	
Distance to rivers - large	m	Canada	NRCan (2019)	1:15000000	NA	
Distance to rivers - medium	m	Canada	NRCan (2019)	1:5000000	NA	
Distance to rivers - small	m	Canada	NRCan (2019)	1:1000000	NA	
Exposure proxy	-	Canada	This study	200 m	NA	
SPM (surface)	g/m ³	Global	Copernicus (2022b)	4 km	2007 —	
Wave velocity (seafloor)	m/s	Arctic	Copernicus (2022a)	3 km	2007	
,		Global	Copernicus (2022c)	0.2°	2007	
Mean current velocity	m/s	BC	Peña et al. (2019)	3 km	2007 -	
(apofloar)		Salish Sea	SalishSeaCast ERDDAP v19-05*	500 m	2007	
(seanoor)		Arctic & Atlantic	ANHA12 (Hu et al., 2019) [†]	0.0833°	2007	
Temperature (seafloor)	°C	BC	Peña et al. (2019)	3 km	2007 -	
,	°C	Salish Sea	SalishSeaCast ERDDAP v19-05*	500 m	2007	
	°C	Arctic & Atlantic	ANHA12 (Hu et al., 2019) [†]	0.0833°	2007	
Salinity (seafloor)	ppt	BC	Peña et al. (2019)	3 km	2007 -	
	TT -	Salish Sea	SalishSeaCast ERDDAP v19-05*	500 m	2007	
		Arctic & Atlantic	ANHA12 (Hu et al., 2019) [†]	0.0833°	2007 —	
Ice thickness (surface)	m	Arctic & Atlantic	ANHA12 (Hu et al., 2019) [†]	0.0833°	2007	
Ice concentration (surface)	%	Arctic & Atlantic	ANHA12 (Hu et al., 2019) [†]	0.0833°	2007 —	
Dissolved oxygen (seafloor)	mol/m ³	Global	Bio-ORACLE V2.2 (Assis et al., 2018)	0.0833°	2000 -	
Primary production (surface)	a/m ³ /d	Global	Bio-ORACLE V2.2 (Assis et al., 2018)	0.0833°	2000 -	
Chlorophyll concentration	mg/m ³	Global	Bio-ORACLE V2.2 (Assis et al., 2018)	0.0833°	2000	
(surface)	5		(2014	
Max current velocity	m/s	Global	Bio-ORACLE V2.2 (Assis et al., 2018)	0.0833°	2000	
(seafloor)					2014	

191 Notes: BC = British Columbia; BPI = Benthic position index; VRM = Vector ruggedness measure; SPM = Suspended

192 particulate matter. *See <u>https://salishsea.eos.ubc.ca/erddap/index.html</u>; Soontiens and Allen (2017); Soontiens et al.

193 (2016). [†]See: <u>https://canadian</u>-nemo-ocean-modelling-forum-community-of-

194 practice.readthedocs.io/en/latest/Institutions/UofA/Configurations/ANHA12/index.html

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197 2.3 Predictor variables

198 <u>2.31.1-2 Benthic terrain features</u>

199 A set of 10 benthic terrain features were constructed from the unified bathymetric layer (Table 1). As benthic terrain measures use data on the depth of a location relative to the depth of 200 201 surrounding cells up to a given distance, bathymetric data within a given buffer outside the study area maxima were included as needed to avoid edge effects in each terrain feature. Slope and 202 total curvature were calculated using the terra.terrain (Hijmans, 2022) and spatialEco.curvature 203 204 (Evans and Murphy, 2021) functions respectively. As these measures can be particularly sensitive 205 to artifacts from the DEM models and projections, they were constructed at two resolutions - the native 200 m resolution, and after aggregating the bathymetry by 5-fold to 1 km x 1 km (termed 206 207 "smoothed"). Smoothed layers were disaggregated back to a 200 m resolution to maintain 208 uniformity across predictor layers.

209 Benthic position index (BPI) and vector ruggedness measures (VRM) were each calculated using 210 the MultiscaleDTM package at 3 different levels to capture both small local features and larger 211 spatial variation in terrain -(Maxwell and Shobe, 2022; Ilich et al., 2021). Benthic position index 212 was calculated as the difference between the depth of a focal cell and the mean of cells contained 213 in annulus shaped window of 0.2 km to 5 km (BPI fine), 2 km to 25 km (BPI medium) and 4 km to 100 km (BPI broad). Vector ruggedness was measured by considering variation in the depth 214 215 surrounding each cell within square windows of width 1 km (VRM fine), 5.8 km (VRM medium) 216 and 11.6 km (VRM broad). Due to extremely inhibitive computational times when calculating VRM broad, BPI medium and BPI broad at 200 m resolution, for these features the bathymetric layer 217 was first aggregated to a 400 m resolution before feature calculation, and then disaggregated 218 back to 200 m to maintain uniformity. 219

220

221 <u>2.31.2-3 Predictors describing the geographic setting</u>

The geographic setting of each cell was described by its distance to shore and rivers, its broad bioregional classification, and a proxy measure <u>for exposure</u> describing the degree of exposition vs. shelteredness (Table 1). The geographic setting features are also influenced by the values of surrounding pixels, therefore appropriate buffers were also applied to the processing of these layers to avoid edge effects. Distance to shore was measured by the Euclidian distance to the nearest land cell (indicated by an 'NA' value in the bathymetry layer), while bioregion was defined by the Fisheries and Oceans Canada Federal Marine Bioregions classification (DFO, 2022). The
bioregion polygons were edited to include all bathymetry cells and re-classified with an integer
scale of 1 to 12 from east to west.

231 CanVec is a digital cartographic reference product produced by Natural Resources Canada (NRCan) which includes the location of rivers across Canada at three mapped scales (NRCan, 232 233 2019). Firstly, the coarsest scale data (1:15,000,000) was projected onto the CRS of the bathymetry layer and converted from polylines to a 2 km resolution raster. A 2 km buffer was 234 235 added around each river to ensure overlap of river mouths with the bathymetry data. The resultant raster layer was resampled onto the bathymetry raster and the grid distance of each bathymetry 236 237 cell to the nearest river-mouth cell was calculated using the terra.gridDist function (Hijmans, 238 2022). This was then repeated for the medium scale (1:5.000.000) and fine scale (1:1.000.000) layers with each river raster overlayed with the previous coarser scale layer to ensure all rivers 239 240 were included as the scales decreased.

241 To approximate the exposure setting of each cell, data on the mean distance from shore of 242 surrounding cells was used to construct a proxy value of fetch. Using the terra.focal function 243 (Hijmans, 2022), the mean distance to shore of surrounding pixels was calculated in square 244 windows of width 10 km, 20 km, 50 km, 100 km, 175 km and 250 km. Due to extremely inhibitive 245 computational times when calculating these values at the two largest distances, the distance to 246 shore layer was first aggregated to a 400 m resolution before focal calculations of these 247 components, and then disaggregated back to 200 m to maintain uniformity. The maximum value in each layer was then set to the relative window size, and all data in each layer normalised 248 between 0 and 1. The mean of all layers was then calculated which resulted in continuous 249 250 measure of relative exposure/shelteredness ranging from 0 (highly sheltered) to 1 (highly 251 exposed).

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253 <u>2.31.3-4 Satellite derived predictors</u>

Using data from the Copernicus Marine Data Store, two layers were created approximating the mass of suspended particulate matter in surface waters and the orbital velocity of waves at the seafloor. Data on suspended particulate matter <u>(SPM)</u> in surface waters across Canada from 2007 to 2019 was extracted in netCDF format from ACRI-ST (Sophia Antipolis, France) company's global Bio-Geo-Chemical products at 4 km spatial resolution and a monthly temporal resolution (Copernicus, 2022b). The climatological mean across this entire period was then

260 calculated for each cell and the netCDF converted to a raster for further processing. Due to the 261 complex nature of the Canadian coastline and the large dissimilarity disparity in spatial resolution 262 of the satellite data product (4 km) and the layers created above (200 m), the satellite raster layer was allowed to extrapolate by 1 cell in its native resolution by taking the mean value of 263 neighbouring pixels. This allowed better overlap of satellite layers with the study area maxima at 264 the coastline but limited over-extrapolation. The raster layer was then reprojected to the equal 265 266 area CRS and resampled onto the bathymetry layer using cubic-spline interpolation. Due to a lack 267 of consistent SPM data recorded in the northern Arctic Basin, this portion of the data layer was manually removed within QGIS. 268

269 To calculate the estimated orbital velocity of waves at the seafloor, two satellite wave data 270 products were combined with the unified bathymetry layer as constructed above. Hourly data from 2007 to 2019 on the significant wave height (H_s ; VHM0) in meters, and primary wave swell mean 271 period (T_z ; VTM01 SW1) in seconds, were extracted from the 0.2° resolution Global Ocean Wave 272 273 Reanalysis (WAVERYS) produced by Mercator Océan International (Copernicus, 2022c) and the 274 3 km resolution Arctic Ocean Wave Hindcast produced by MET Norway (Copernicus, 2022a). All 275 data were processed as the SPM data layer (except for lack of removal of the Arctic basin data), 276 and converted to an estimate of orbital wave velocity at the seafloor (U_{rms} ; measured in m s⁻¹) using the following equation from Soulsby (2006): 277

278
$$U_{rms} = \left(\frac{H_s}{4}\right) \left(\frac{g}{d}\right)^{0.5} \exp\left\{-\left[\left(\frac{3.65}{T_z}\right) \left(\frac{d}{g}\right)^{0.5}\right]^{2.1}\right\}$$
(1)

where *g* is the acceleration due to gravity (9.806 m/s²) and *d* is the water depth (m), taken as the unified bathymetry layer multiplied by -1, and all values less than 1 meter depth rounded up to the nearest meter (as needed for the above calculation). The resultant Arctic orbital velocity data layer was then bias corrected to the global orbital velocity data layer utilising the *qmap* package with quantile mapping using a smoothing spline (Gudmundsson et al., 2012). Finally, the two data layers were overlayed with the regional Arctic data taking priority over the global data where available.

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287 <u>2.31.4-5 Ocean circulation model predictors</u>

<u>To incorporate best available regional evidence</u>, <u>Dd</u>ata on the mean surface ice cover, seafloor
 salinity, temperature and current velocity was collated from three different ocean circulation model
 products covering different regions of Canada (Table 1: see Appendix A3 for further details).

291 ANHA12 is a regional configuration of the NEMO ocean and sea-ice model (Madec et al., 1998) 292 created at the University of Alberta, covering the Arctic and northern Hemisphere Atlantic at 5 day 293 temporal resolution, a curvilinear 1/12th degree horizontal resolution ranging from 1.93 km in the Arctic to 9.3 km at the equator, and 50 vertical levels (Hu et al., 2019). The British Columbia 294 295 continental margin (BCCM) circulation model created by Fisheries and Oceans Canada (DFO) 296 covers the entire Canadian Pacific coast and extends approximately 400 km offshore. It has a uniform horizontal resolution of 3 km, 42 vertical levels and a 3 day temporal resolution (Peña et 297 al., 2019; Masson and Fine, 2012). As the BCCM model has higher uncortainty in nearshore and 298 299 enclosed environments due to its relatively coarse resolution, data was also extracted from the Salish Sea Cast ERDDAP data server. Similarly to the ANHA12 model, the Salish Sea Cast is a 300 configuration of the NEMO circulation model developed by a consortium of Canadian Universities 301 and government agencies and extends from Juan de Fuca Strait to Puget Sound to Johnstone 302 Strait at 500 m horizontal resolution, 40 vortical layors and hourly temporal resolution (Seentions 303 and Allen, 2017; Soontiens et al., 2016). For further details on all these models, see relevant cited 304 references. It should be noted that many of these ocean circulation models contain high 305 306 uncertainty in nearshore areas. However, they are expected to be greatly improved when 307 compared to global circulation model products which are frequently used in this sort of predictive mapping work (e.g. Atwood et al., 2020; Lee et al., 2019; Assis et al., 2018). 308

309 _Three-dimensional data for salinity, temperature, u-velocity (eastward) and v-velocity (northward) was-were extracted from each model and the climatological mean across all time points between 310 2007-2019 was calculated. For each horizontal cell, data were only retained from the lowest 311 312 vertical cell within a given position (i.e. the cell which contacts the seafloor) value was taken as 313 the lowest vertical cell within a given position. Individual model outputs were then converted to 314 spatial point data using the cell centroid positions and transformed to the unified equal area-CRS. Point data was then converted to rasters with the respective resolution of each model, and the 315 mean value taken if two points from the same model lay within a single raster cell as an artifact 316 of reprojection. As the Arctic-Atlantic model (ANHA12) model has a varying horizontal resolution, 317 point data were rasterized using the smallest resolution of the original model (1.6 km) and then 318 interpolated using the *gstat* package (Gräler et al., 2016) and a nearest neighbour interpolation 319 320 method (including cells for land within the original model grid to supress extrapolation). For all 321 three models, mean current velocity was then calculated as the root mean square of the u-velocity 322 and v-velocity values in each cell. Finally, as carried out for the satellite data layers, each raster 323 was allowed to extrapolate by one cell in its native resolution (or for the case of the ANHA12 model -____ its median resolution) and resampled onto the 200 m bathymetry grid using cubic-spline 324

325 interpolation. The three rasters were then combined with data only being assigned to the spatial 326 extent of the respective bioregions as defined in Section 2.1.3.; the Salish Sea Cast data only 327 being applied to cells that lay within the Salish Sea bioregion (as calculated in Section 2.3.2), the 328 BCCM model outputs only being assigned to other bioregions within the Pacific and ANHA12 329 used for all Atlantic and Arctic regions. Although this means that different model products were used to measure the same predictor variable in different regions, which can create biases, the 330 331 bioregion predictor variable was included as a co-variate in all models which included the ocean circulation variables, thus allowing for interactive effects and accounting for differences in 332 333 circulation model structures. Combining different models can also create edge-effects, however the Arctic-Atlantic model is entirely spatially distinct so contains no common edges with other 334 models. The only significant edge between the remaining two models lies at the mouth of the 335 336 Juan de Fuca Strait and minimal disparity was seen (with the other common edge occurring in the narrows of Johnson Strait). 337

Predictor layers describing the mean concentration and thickness of sea ice for the same temporal period across the Arctic and Atlantic were also derived from the ANHA12 model. Processing of model data and spatial rasters was conducted as above, except a value of zero ice concentration and thickness was applied to all cells across the British Columbia Pacific bioregions.

342

343 <u>2.31.5-6 Global model predictors</u>

Four additional predictor variables were derived from Bio-ORACLE version 2.2 - a global unified 344 345 marine environmental data-layers collation which gives climatological mean values at 1/12th 346 degree resolution, for 2000-2014 and a wide-range of environmental variables (Assis et al., 2018). 347 Although these datasets are expected to be of lower accuracy of lower resolution when compared 348 to the regional data used above, based on previous research there were some additional variables 349 not available from the regional circulation models which were considered potentially important for 350 carbon modelling (Diesing et al., 2021; Atwood et al., 2020). Three described the oceanographic 351 chemistry/biology - namely primary production and chlorophyll content of the surface water column, and dissolved oxygen concentration at the seafloor. The fourth predictor was an 352 353 additional measure of current velocity (maximum current velocity), which was selected on top of the previously derived mean values because current velocity has been identified as a particularly 354 strong predictor within previous seafloor sediment composition and carbon content predictive 355 356 mapping studies (Gregr et al., 2021; Diesing et al., 2021; Mitchell et al., 2019). Raster data were

downloaded from the Bio-ORACLE website and processed as the satellite data layers (i.e. allowed to extrapolate by 1 cell in its native resolution by taking the mean value of neighbouring

pixels, reprojected to the unified equal area CRS and resampled to the unified 200 m grid using
 cubic-spline interpolation).

361

362 2.31.6-7 Final collation of predictor variables

The resulting 28 predictor variable raster layers were combined into a single raster stack and any cells containing NA values removed, leaving only those cells which contained values across all predictor layers. The remaining cells covered 92.3% of the subtidal zone of the Canadian EEZ and delineated the maximum potential modelling area (Fig. 1). The final predictor variable layers are shown in the Supplement.

368

369 2.4-2 Sediment composition mud content data

370 Sediment composition point data were extracted from two sources. Firstly, all data were exported from the NRCan Expedition Database on 11th November 2022. This data repository contains 371 372 information related to marine and coastal field surveys conducted by or on behalf of the Geological Survey of Canada from the 1950s to present, which deployed sampling methods including piston 373 cores and grab samples. Data were also extracted from a recent synthesis of grain size 374 375 distribution measurements from the Canadian Pacific seafloor (1951-2017), compiled by Geological Survey Of Canada and NRCan (Enkin, 2023). Although there are some duplications 376 377 between these two datasets, these are accounted for in the proceeding pre-processing steps. In 378 both sources, grain size data is reported as the percentage content of mud (sometimes separated 379 into silt and clay), sand and gravel within each sample. Due to modern developments in grain size 380 analyses (e.g. laser diffraction) older samples may have lower measurement accuracy; however, due to the relatively coarse metric being used in this study (%mud/sand/gravel) and the 381 382 occurrence of a number of largescale geological surveys occurring during the 1960s, we chose to retain data from 1960 onwards. Where sampling year was not recorded within the database. 383 384 the date was inferred from the expedition code or from expedition metadata. The sampling method and depth of the sediment from which the sample/sub-sample originates are also predominantly 385 recorded within the database. Where sediment depth was absent, but the sampling method was 386 387 noted as "grab" or "othor", the penetration depth was assumed to be 10 cm (a commonly assumed

388 penetration of standard sediment sampling devices such as Van Veen Grabs and Day Grabs). 389 Empirical point data on seabed sediment mud content across the Canadian EEZ were extracted 390 from two sources (Enkin, 2023; NRCan, 2022) (see Appendix A4 for further information). Samples 391 Data were only retained if they originated from within the top 30 cm of the sediment and had associated geographic position information (latitude-longitude co-ordinates; lat-lon). Data were 392 393 further filtered by excluding those where the sum of mud, sand and gravel content was greater than 102% and lower than 98% - to allow for rounding errors but to exclude invalid data. Data 394 395 were also excluded if samples/sub-samples were not present from at least the top 1 cm to 5 cm below the sediment surface within a given sampling event. After data filtering, the mean 396 397 percentage of mud was taken across replicates/sub-samples, leaving a single value for each 398 sampling event. We chose to concentrate on sediment mud content as this has previously been 399 identified as the key sediment composition component from a number of related carbon mapping studies (Smeaton et al., 2021; Diesing et al., 2017, 2021; Pace et al., 2021; Wilson et al., 2018). 400 401 Finally, mud content data were projected onto the CRS of the predictor layers and only retained 402 where overlap occurred. This led to a final dataset of 19,730 samples (Fig. A1B1).

403

404 **2.5-3 Organic carbon content data**

405 <u>2.53.1 Organic carbon data collation and extraction</u>

Data on the percent organic carbon content within dried surface sediments (%OC) was collected from three different structured searches. Firstly, a systematic literature review was conducted through Web of Science and Scopus. Both searches were conducted on the 21st September 2022. Within Web of Science, its "Core collection" was searched via the field "Topic", which examines a paper's title, abstract, author, keywords and "keywords plus". Within Scopus, the search was run via the field "Title-Abs-Key", which scans a paper's title, abstract and keywords. Within both databases the same search string was used:

413 ("organic carbon" OR "organic matter" OR "organic content" OR TOC OR TOM) AND (coast* OR
414 sea* OR ocean* OR estuar* OR marine OR gulf) AND (sediment* OR mud* OR sand* OR clay*
415 OR silt* OR gravel* OR seabed) AND Canad*

All articles identified from the searches were exported into a single Zotero library and duplicates removed, leaving 1,581 results. Screening was conducted via a hierarchical process that first assessed the title, then abstract and finally full text. At each stage an article was assessed against the inclusion criteria described below, with those considered relevant or of unclear relevancepassing to the next level of assessment.

421 The inclusion criteria were defined as: 1) Study conducted on subtidal seabed sediments (those 422 concerning rock, shale or fauna were not included); 2) Physical samples collected using a seabed 423 sediment sampling device (e.g. cores or grabs - sediment-trap samples were not included); 3) Samples from within the Canadian EEZ; 4) Studies concerning the chemical composition of the 424 sediment; 5) Organic carbon content (%) directly measured after separation of organic and 425 426 inorganic components (e.g. by acidification). After the title screening stage 242 articles remained, followed by 123 remaining after abstract screening, and a final set of 49 articles left for data 427 428 extraction after review of the full text. Four additional primary literature papers were added based 429 on expert advice. This included two large data collation studies, one concentrating on the Arctic 430 (CASCADE; Martens et al., 2021) and one having global scope (MOSAIC v2; Paradis et al., 2023)

431 The second structured search was conducted on the Canadian Federal Science Libraries Network 432 - a repository which contains departmental publications, reports and data sets from seven science-based Canadian government departments. The search was carried out on the 7th 433 434 November 2022 using the same search string as for the primary literature and querying all fields. 435 The search led to only 178 results and therefore each result was assessed individually against 436 the selection criteria first by their abstract and then by a full text assessment, leading to data 437 extraction from 15 reports. The third search was carried out on the 15th November 2022 using GEOSCAN - the NRCan bibliographic database for scientific publications. As GEOSCAN does 438 439 not allow search strings containing "AND", the search was conducted on all fields using only the terms: "organic carbon" OR "TOC" OR "OC"; leading to 655 search results. The metadata of all 440 441 entries was exported as a text file and further refined using a secondary manual search for the 442 remainder of the search terms listed above within Microsoft Excel. This led to a final set of 233 results, 178 which were excluded by screening of the title, and a further 51 excluded by abstract 443 444 or full text screening, leaving 4 reports for data extraction.

In total, these three structured searches of primary literature and government reports led to 72 individual entries publications for data extraction. As well as data on the %OC, metadata extracted included the maximum depth of sample into the sediment (cm), geographic position (lat-lon), sample ID, year of sampling (approximated as publication year where not clearly stated), sampling method (e.g. multicorer, Van Veen grab) and water depth of sample site (where recorded). Data were extracted from data tables or supplementary databases when available, otherwise the PlotDigitizer online application was used to extract data from graphical products. Where possible data were extracted on the %OC in different depth-layer sub-samples through a single core-sample up to 50 cm, otherwise a single mean value was taken.

454 Additional to data collated through the structured searches, %OC data were also extracted from 455 PANGAEA - a global data repository for geographic earth-system data (PANGAEA®, 2022). A data search across all topics was conducted on the 25th October 2022 using the same search 456 terms as for the structured search, except for removal of the term "Canad". The geographic 457 extent of the results was instead delineated using the spatial tool within PANGAEA which allows 458 459 results to be filtered by the geographic co-ordinates of a square/rectangular extent. Overall, this led to a total of 1,489 potential datasets. All relevant data within these datasets were exported 460 461 using the Data Warehouse Download tool within Pangaea. Based on expert knowledge, two additional PANGAEA datasets were added to the output from published global %OC data-462 syntheses (Atwood et al., 2020; Seiter et al., 2004). Lastly, where the date of the sample was not 463 recorded, the sampling year was manually added by further exploring the metadata or cited 464 465 studies. To align the PANGAEA data with the systematic review data, PANGAEA data points 466 were excluded if: 1) they lacked data on %OC; 2) they lacked metadata on the depth of a sample 467 within the sediment; 3) if the sample originated from greater than 50 cm below the sediment 468 surface; or 4) metadata on the elevation/water depth indicated sampling above the subtidal. Additionally, metadata within PANGAEA were coalesced where necessary (due to different 469 470 names being given to the same data type), and mean values of %OC taken if replicates were measured within a single sub-sample. 471

All organic carbon data were converted into spatial point data, transformed to the unified equal 472 area CRS and masked by the predictor variable's maximum model area to leave only overlapping 473 474 data. Additionally, values were only retained from the sampling year 1959 and onwards. The extra 475 year was included when compared to the sediment composition mud content data because there 476 were some widescale surveys undertaken across the Labrador Sea in 1959 which was lacking 477 from any additional %OC datasets. While this large temporal extent may add uncertainty in relation to the quality and uniformity of the response data, similar extents have been used by 478 previous global mapping studies (Atwood et al., 2020; Lee et al., 2019; Seiter et al., 2004) and, 479 480 72% of the %OC data within this study were sampled after 1980 and 55% after 2000. The larger 481 temporal extent also allows for the inclusion of a larger frequency and wider spatial extent of data, 482 therefore potentially improving accuracy robustness in of our spatial predictive modelsens. In total 483 our %OC dataset contained 2,518 point-samples (Fig. A2B2) and 3,308 sub-samples across 484 different depth layers within cores.

486 <u>2.53.2 Organic carbon data processing</u>

487 Due to commonly adopted uneven sampling distributions within single core samples (i.e. more 488 sub-samples towards the top of the core), where sub-sample data were present on the %OC in 489 different depth-layers these were converted into weighted cumulative means assuming linear distribution between sub-samples. Additionally, there was large variation in the maximum 490 sediment depth of point-samples, ranging from %OC measures from only the top 1 cm of 491 492 sediment, to values up to the chosen data extraction limit of 50 cm deep. We chose to standardise 493 all samples to 30 cm depth as only 6% of the point-samples covered sediment depths below this layer and because 30 cm is a commonly suggested carbon stock accounting depth for terrestrial 494 495 soil and marine sediment habitats in both carbon accrediting methodologies and greenhouse gas 496 inventories (VERRA, 2020; IPPC, 2019).

497 To estimate the cumulative mean of %OC at 30 cm for all individual point-samples, we created a 498 transfer function using a generalised additive mixed model (GAMM) smoothing spline. It is 499 generally expected that the %OC in marine sediments decreases with depth within the seafloor 500 (Middelburg, 2018); we used the collated data above to approximate a mean decay function trend 501 for this study. Firstly, only those data that contained at least five sub-sampled depth layers were 502 retained for modelling as fitting distributions to those with fewer points would likely be invalid. This 503 left 183 unique samples with 2,640 weighted cumulative mean sub-samples for model 504 construction. Cumulative mean %OC data were arcsin transformed (arcsin{ $\sqrt{[\% OC/100]}$; a 505 commonly adopted transformation for percentage data), and a simple GAMM model applied with sub-sample sediment depth as the fixed factor modelled with a cubic regression spline and 506 507 sample ID as the random factor. The GAMM model was fitted using the macv package; a scaled-508 t distribution family was used for heavy tailed Gaussian-like data, the number of basis dimensions was set to 20 and smoothing parameter estimation was conducted by Restricted Maximum 509 Likelihood (REML) (Wood et al., 2016). Model validation was carried out using visual assessment 510 511 of diagnostic plots of residuals, as well as observed vs fitted values. Significance of the sampling 512 depth smoothing spline was assessed by an analysis of variance (ANOVA) with a chi-squared 513 test comparing the full GAMM model to a null GAMM model containing only the random factor 514 and the intercept (see Appendix B-C for results). The difference between estimated deviance explained in the full and null models was also used to approximate the variance explained by the 515 516 fixed and random factors. To create a transfer function, the cumulative %OC was predicted from 517 the mean fixed effects of the GAMM model at sediment depths from 0 - 30 cm at 0.1 cm intervals.

The predictions were then back-transformed to percentage data and the cumulative mean %OC at each depth was converted to an inverse proportion of the mean <u>acrossat</u> 30 cm. Overall, this gave an estimated proportional conversion factor from the cumulative mean at any given depth to an expected <u>cumulative</u> mean <u>at across</u> 30 cm (Appendix <u>BC</u>).

All point-sample data from PANGAEA and the systematic review were combined, corrected to weighted cumulative means where sub-samples were present, checked for duplication, and unified to a mean %OC value of the top 30 cm of sediment using the above transfer function. One outlier was removed from the dataset as it was reported to have a carbon content twice that of any other sample within the dataset. Finally, for further analyses %OC data were arcsin transformed due to a highly right skewed distribution and its application within similar modelling exercises (Smeaton et al., 2021; Diesing et al., 2017).

529

530

531 2.6-4 Final model domain selection

After visual assessment of the coverage of both the <u>sediment compositionmud content</u> and %OC data, the final model domain was limited to a water depth of 2,500 meters. This depth limit (as delineated by the bathymetry predictor layer) encompassed 99.95% of <u>sediment compositionmud</u> <u>content</u> point data (Fig. A1B1) and 99.3% of %OC data (Fig. A2B2). The predictor layer raster stack was filtered with all cells deeper than 2,500 meters excluded from the model domain. This final model domain covers 4,489,235 km² which is 78.4% of the EEZ or 92.6% of the seafloor area above 2,500 m (Fig. 1).

539

540 2.7 Sediment mass accumulation rate data

541 From preliminary exploratory research it was determined that there would be insufficient data on 542 organic carbon accumulation rates, or sediment mass accumulation rates, to undertake a 543 Canada-specific data synthesis. We therefore chose to downscale a recent global spatial 544 predictive map of seafloor sediment mass accumulation rates (Restreppo et al., 2021). To approximate a sample of values across the model domain in this study the global mass 545 546 accumulation rate data (MAR; log₁₀{g cm⁻² yr⁻¹}) netCDF was converted to a raster and masked 547 by the coverage of the model domain. The raster layer was then converted to spatial point data by the location of cell centroids, and a stratified-random sample of 10% of the data was taken. 548

549 Data was stratified by assigning the x-coordinate, y-coordinate and mass accumulation rate 550 values to decile bins; and a random sample of 10% of values taken within each unique 551 combination of the three-way binning. This resulted in 12,660 point estimates of MAR across the 552 model domain, which were then reprojected to the unified equal area CRS for further analyses 553 (Fig. A3).

554

555 2.8-5 Random forest modelling

For predictive mapping we adopted random forest machine learning techniques due to their 556 flexibility regarding violations of traditional statistical assumptions, ability to handle a range of data 557 558 types and predictor variables and elucidate both drivers of model response and predictions of 559 uncertainty, as well as their successful application in previous similar modelling tasks (Diesing et 560 al., 2017, 2021; Pace et al., 2021; Atwood et al., 2020; Wilson et al., 2018). Contemporary 561 research in spatial machine learning techniques have highlighted that rebust spatially explicit cross-validation (CV) strategies and predictor variable selection processes are essential to 562 563 calculate valid performance metrics, limit overfitting and construct reliable spatial predictions (Zhang et al., 2023; Ludwig et al., 2023; Meyer and Pebesma, 2022; Meyer et al., 2019). We 564 565 discuss the incorporation of these processes into our modelling framework below.

566 Three response variables (mMud content and, organic carbon content (%OC) and MAR) were 567 both modelled using the following framework. Firstly, each response variable was overlain onto the predictor variable grid and the mean values were taken if more than one data-point fell within 568 569 a single raster cell. All predictor variable data were then extracted for each response dataset; 570 however, the three biological/biochemical predictor variables (primary production, chlorophyll concentration and dissolved oxygen) were only used within the %OC model as they are not 571 572 expected to drive variation in physical sediment properties (Restreppo et al., 2021; Gregr et al., 573 2021; Graw et al., 2021; Mitchell et al., 2019).

574 <u>Contemporary research in spatial machine learning techniques have highlighted that robust</u> 575 <u>spatially-explicit cross-validation (CV) strategies and predictor variable selection processes are</u> 576 <u>essential to calculate valid performance metrics, limit overfitting and construct reliable spatial</u> 577 <u>predictions (Zhang et al., 2023; Ludwig et al., 2023; Meyer and Pebesma, 2022; Meyer et al.,</u> 578 <u>2019). We discuss the incorporation of these processes into our modelling framework</u> 579 <u>below</u>Details of the methods used to ensure appropriate cross-validation design and feature 580 <u>selection are discussed in Appendix A5.</u>

For each response variable, the spatialsample package (Silge and Mahoney, 2023) was used to 581 582 construct a variety of spatial CV data-fold structures (splitting the data into different analysis and 583 assessment sets) and the validity of each structure was visually assessed using the 584 CAST.plot_geodist function (Meyer et al., 2023). This function creates density plots of nearest 585 neighbour distances in multivariate predictor space between all response data as well as between 586 response data and a random sample of prediction locations, and between analysis and 587 assessment data within CV folds (see Appendix C). The suitability of a given CV structure to be 588 representative of estimating map accuracy can be determined by visually assessing the density 589 plots and finding the analysis-to-assessment CV-distance curve being closely aligned to the 590 sample-to-prediction density curve (see Appendix D; Ludwig et al., 2023; Meyer and Pebesma, 591 2022). Contrastingly, if the sample-to-sample distance curve closely overlays the sample-to-592 prediction curve, this indicates that traditional random cross-validation strategies are likely to be 593 appropriate (see Appendix D; Ludwig et al., 2023). To approximate sample-to-prediction 594 distances, the sample size number within *plot_geodist* was set to select 5,000 random samples across the model domain. Further, as the spatial distribution of data is a key consideration to 595 596 ensure robust cross-validation (Ludwig et al., 2023; Meyer and Pebesma, 2022), the x- and y-597 coordinates of each data point were also included as predictor variables in the plot_geodist 598 calculations.

599 For the mud content data, a spatial kmeans clustering CV structure was chosen as the response 600 data had good coverage of the model domain, contained a large number of data points, and 601 showed relatively strong spatial clustering (Fig. A1). A range of options in the number of kmeans 602 clusters were tested, with 35 being determined as the optimal number and each cluster being 603 assigned to its own CV fold (Fig. C1). Through visual assessment of the density plots, it was 604 identified that the kmeans CV structure was somewhat mis-aligned from response-to-prediction 605 distances, with the CV distances being overly conservative at including near-distance comparisons (Fig. C1). We therefore used a partially repeated CV strategy, with a small number 606 607 of randomly selected data-points added to the assessment set in each kmeans spatial-CV fold 608 (1% of mud content data randomly sampled at each fold without replacement) (Fig. C2). As the 609 %OC response dataset was relatively small and spatially dispersed (Fig. A2), we used a spatial 610 block CV strategy in place of the kmeans clustering to avoid clusters containing highly spatially dispersed data. We chose to use hexagonal shaped blocks, random assignment of blocks to folds, 611 612 and the same number of CV folds as for the mud content data (v = 35) - both to maintain uniformity and because varying the fold-number did not significantly influence the density plots. Instead, the 613 614 diameter of the spatial blocks was altered, and an optimal block size of 100 km identified using 615 the *plot geodist* function (Fig. C3). For both response variables, following identification of an 616 appropriate CV35-fold spatial CV structure, a single fold was assigned held-back as testing data, 617 with all other data retained for model fittingtraining. To ensure an absence of duplication between the training and testing data, Following the training-testing split, the 34 spatial CV folds were 618 619 reconstructed on the training data (i.e. all training data assigned to one of 34 validation sets). on 620 the training data to ensure an absence of duplication. For the MAR data, the density plots 621 indicated that traditional random cross-validation would be a valid approach (Fig. C4), which was 622 expected as the response data were a stratified-random sample across the model domain (Fig. 623 A3). The random CV folds were stratified by the MAR response value to ensure a relatively even distribution across CV folds. A 10% stratified-random sample was first assigned as the test-set 624 625 and random CV folds assigned to the remaining training data.

Three random forest models were constructed (mud content, OC content and MAR), each 626 following the same modelling protocol. Firstly, tUsing these CV folds, the CAST.ffs function 627 628 (Meyer et al., 2023) was then used to run a spatially-explicit forward predictor variable selection processes with appropriate spatial considerations (see Appendix A5 for further information). The 629 630 function fits a model with all combinations of two-way predictors, selects the best model based on 631 a given metric, and then increases the number of predictors by one, testing all remaining 632 variables. This iteratively continues with the process stopping if none of the tested variables 633 increases the performance when compared to the best previous model with "n-1" predictors. The function also allows models to be fit separately across all individual CV folds, therefore 634 incorporating appropriate spatial considerations into the feature selection process. Due to the 635 large number of variables within this study, and the relatively large datasets, this process was 636 very computationally expensive. We therefore chose to adapt the function to initiate forward 637 variable selection after a priori identification of the first two predictor variables. These variables 638 639 were identified by constructing a basic random forest model with all training data and predictor variables, and the hyperparameters mtry (the number of variables to randomly sample as 640 candidates at each split), min n (the number of observations needed to keep splitting nodes) and 641 642 trees (the number of random forest trees to construct and take mean predictions across) set to 2, 5 and 1.000 respectively. Variable importance was estimated using permutation, and the two 643 644 predictor variables with largest importance selected. The ffs function was then run starting with the two pro-selected variables (see Fig. 3, 6 & 9) and performance of each iteration assessed on 645 646 the root mean squared error (RMSE) of predictions across all CV folds.

647 Following variable selection, hyperparameter tuning was conducted on the hyperparameters mtry 648 (the number of variables to randomly sample as candidates at each split) and min_n_min_n (the 649 number of observations needed to keep splitting nodes); hyperparameters, with the number of trees hyperparameter (the number of random forest trees to construct and take mean predictions 650 across) set to 1,000 (Probst et al., 2019). 11 potential combinations of hyperparameters were 651 652 selected using a semi-random Latin hypercube grid (Kuhn and Silge, 2023; Kuhn and Wickham, 653 2020). The tuning process fitted individual separate models across all CV folds and hyperparameter combinations - each with 11 combinations of hyperparameters (i.e. 34 CV folds 654 655 x 11 hyperparameter options = a total of 374 models) which were selected using a semi-random Latin hypercube grid(Kuhn and Silge, 2023; Kuhn and Wickham, 2020). The performance of each 656 of the 11 hyperparameter combinations was assessed based by on-calculating the root mean 657 squared error (RMSE) of on predictions of the validation data across all CV folds, with the optimal 658 hyperparameter combination selected as that with the lowest RMSE s(Meyer et al., 2019, 2023). 659 660 After selection of the best performing hyperparameter combination, a single last-fit model fit-was conducted constructed on the entire training set and evaluated on the held-back test set (Kuhn 661 and Silge, 2023; Kuhn and Wickham, 2020), with the absence of overfitting determined by the 662 663 RMSE and R² of the last-fit model falling within the range of those found across CV folds with 664 optimal hyperparameters. Overall Final model performance metrics (RMSE and R²) (RMSE and 665 R²)-were then calculated using the all predictions of validation data across from all-CV folds (with 666 optimal hyperparameters) folds with optimal hyperparameters and from predictions of the testing 667 data from the last-fit model (Meyer et al., 2019, 2023).; while predictor variable importance was 668 calculated by fitting an additional model across all training data using optimal tuning parameters and the importance calculated through permutation(for further details see Kuhn and Silge, 2023; 669 Wright et al., 2016). Accumulated local effects (ALE) plots were produced for the six predictor 670 variables with highest importance in each model using the iml package (Molnar et al., 2018) to 671 672 give a visual representation of the average effect of predictors on model prediction outcomes. Finally, mean model pPredicted values redictions were then calculated across the entire model 673 674 domain using the last-fit model and the predictor variable raster stack (Kuhn and Silge, 2023; 675 Kuhn and Wickham, 2020), and cell-specific estimation of uncertainty was calculated using 676 standard error on out-of-bag predictions using infinitesimal jack-knife for bagging (Roy and 677 Larocque, 2020; Wager et al., 2014). Due to computational restraints when calculating predictions 678 across the entire model domain (which contains 112,230,871 cells), data-the predictor variable 679 raster stack werewas split into 150 non-overlapping partitions by random sampling es (without 680 replacement) and both prediction and standard error estimates made serially on each

splitpartition. - All predictions were then merged to create a raster layer covering the entire model
 domain (although edge effects were not expected between partitions, random sampling without
 replacement across the entire domain was chosen to ensure its absence).-

A cell-specific approximation of the upper and lower bounds of the 95% confidence interval (CI) 684 was calculated by adding/subtracting the cell-specific standard error estimates, each multiplied 685 by 1.96, from the mean predictions and then back transformed where needed (Kuhn and 686 Wickham, 2020; Wager et al., 2014). After calculation, CI values were corrected where necessary 687 - being bounded by 0, and where applicable also bounded by 100. The resulting three raster 688 layers from the mud content model were also used as available additional predictor variables 689 when constructing the random forest models for %OC and MAR as outlined above (Fig. 2). 690 Although this gives the potential for data leakage if mud content and %OC data were from the 691 same samples, we found only 31 occurrences (1.3% of OC samples) where direct spatial overlap 692 693 occurred, and therefore do not consider that significant data leakage is present and no impact on 694 variable importance or model performance calculations will be seen. Finally, a measure of relative predictor variable importance was calculated by fitting an additional single random forest model 695 on all training data using optimal hyperparameters, and the predictor importance calculated on 696 697 out-of-bag data through permutation of predictor variable values (for further details see Kuhn and Silge, 2023; Wright et al., 2016). Accumulated local effects (ALE) plots for the last-fit model were 698 699 produced for the six predictor variables with highest importance in each model using the iml package (Molnar et al., 2018) to give a visual representation of the average effect of predictors 700 701 on model prediction outcomes.

702

703 2.9-6 Estimating sediment dry bulk density

704 To An estimate for the dry bulk density of the sediment across the model domain (pD – the mass of dried sediment per unit volume within the seafloor; g cm-3) was constructed across the model 705 706 domain based on the -outputs-predictions of mud content from the random forest model s for mud 707 and organic carbon content were combined with a variety of published transfer functions and 708 global modelled products (Fig. 2). We identified three published functions which describe the 709 relationship between mud content and porosity Three of the transfer functions calculate the 710 porosity of the sediment (Φ ; the proportion of sediment volume which is water) in seabed 711 sediments. based on the predicted mud content using tThe following equations, are respectively from Jenkins (2005), Diesing et al. (2017) and Pace et al. (2021): 712

713	$\Phi = 0.3805. mud + 0.42071$	(2)
-----	--------------------------------	-----

714
$$\Phi = 0.4013. mud + 0.4265$$

715
$$\Phi = 10^{0.138.\log_{10}(mud)} - 0.486$$

Due to each of these equations being approximations of the relationship between mud content and Φ , we chose to take the mean response. In all cases equations mud represents the predicted mean mud content values across the model domain as calculated above, each expressed as a decimal proportion. For Equation 4, mud content was rounded up to the nearest 0.01 as lower values give unrealistic porosity estimates. All <u>sS</u>ediment porosity <u>estimates can</u> were then <u>be</u> converted to an estimate of dry bulk density using the following equation:

722
$$\rho D = \rho S(1 - \Phi)$$
 (5)

where ρS is the grain density of seabed sediments in g cm⁻³, which was set at the frequently used
constant approximation of 2.65 (Diesing et al., 2017, 2021; e.g. Pace et al., 2021; Lee et al., 2019;
Wilson et al., 2018; Kuzyk et al., 2017). Although this standard approximation of grain density is
not ideal, the variation under different environmental settings is generally found to be small when
compared to differences in %OC and porosity, therefore the values of grain density are not
expected to strongly drive variation in organic carbon density (Atwood et al., 2020; Lee et al.,
2019; Middelburg, 2019; Martin et al., 2015; Berner, 1982).

730 To incorporate uncertainty from our mud content predictions, estimates of dry bulk density were 731 also calculated from the cell-specific predictions of the lower and upper bounds of the 95% CI of 732 mud content. We used these derived lower and upper bounds of dry bulk density estimates as 733 best available approximations of uncertainty around the dry bulk density mean estimate values. Equivalent approaches to estimating uncertainty have been used in other seabed sediment 734 735 carbon mapping studies (e.g. Diesing et al., 2017, 2023; Lee et al., 2019). A forth transfer function from Atwood et al. (2020) calculates an estimate of dry bulk density directly from %OC using the 736 737 following equation:

738 pD = 0.861.

(6)

For this equation, carbon content as predicted above was rounded up to the nearest 0.1% as lower values give unrealistic dry bulk density estimates. For each of the four transfer functions (Equations 2,3,4 and 6) the value was calculated using the mean prediction as well as the upper and lower confidence interval bounds of mud content and %OC respectively, resulting in three raster layers from each function.

(3)

(4)

Two further estimates of dry bulk density were calculated using products from global predictive models, both at 5 arc min spatial resolutions. Martin et al. (2015) created a predictive map of seabed sediment porosity, while Graw et al. (2021) estimate sediment wet bulk density (pW) across the global seafloor. Both raster layers were processed as the satellite predictor layers to align with the model domain. The resulting porosity raster layer was converted to dry bulk density using Equation 5, while the wet bulk density layer was initially converted to porosity using the equation:

751 $\Phi =$ (7)

where pSW is the density of seawater estimated as 1.024 g/cm³. In total this led to 14 dry bulk
 density estimates across the model domain. A final mean value and standard error was calculated
 for each cell, and the upper and lower 95% confidence interval bounds calculated using the
 standard error as above.

756

757 **2.10** <u>7</u> Estimating organic carbon standing stock and accumulation rates

758 The organic carbon density (g cm⁻³) is calculated by multiplying the %OC (expressed as a decimal 759 proportion) by the sediment dry bulk density ; while organic carbon accumulation rates (g cm⁻² yr 760 ⁴) are calculated by multiplying MAR by %OC (Fig. 2). For the final calculations, of both density 761 and accumulation the respective means, upper and lower CI-uncertainty bounds were multiplied together to incorporate uncertainty from both components. These compound uncertainties were 762 763 used as best available approximations of the lower and upper bounds of uncertainty around the 764 estimates of mean organic carbon density (akin to Diesing et al., 2017, 2023; Lee et al., 2019). 765 To create a more meaningful response value, s organic carbon density was converted to kg m⁻³ 766 (multiplied by 1000) and organic carbon accumulation to $q m^2 y^4$ (multiplied by 10,000). Finally, 767 the organic carbon stock in each mapped cell can be calculated by multiplying the organic carbon 768 density by the reference sediment depth of this study (0.3 m) and the cell area (40,000 m²) and 769 converted to metric tonnes (divided by 1000). The total accumulation per cell per year can be 770 calculated by multiplying the organic carbon accumulation rate by the cell area. Overall, this allows estimates to be calculated for the total values of organic carbon stock and accumulation 771 across different parts of model domain. 772

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775 **2.11** <u>8</u> Rock substrate distribution case studies

776 The method followed in this study is similar to that used for many similar seabed sediment 777 predictive mapping exercises in that it uses data only from sediment grab and core samples to build predictive maps across the model domain (Restreppo et al., 2021; Graw et al., 2021; Diesing 778 779 et al., 2017, 2021; LaRowe et al., 2020a; Atwood et al., 2020; Lee et al., 2019; Mitchell et al., 780 2019; Wilson et al., 2018; Stephens and Diesing, 2015). One major limitation with this modelling 781 approach is that areas of bedrock, which would have zero values for all sediment response 782 variables, will not be recorded in these datasets. Therefore, the under representation of zero 783 values in the response data could lead to an overestimate of organic carbon standing stocks and 784 accumulation rates as zero values are unlikely to be predicted from model outputs.

785 In the context of this study, information regarding the distribution of bedrock is lacking for many 786 regions. We therefore use two regional case studies from the Pacific British Columbian EEZ and 787 the Atlantic Scotian shelf and slope where recent publications have made estimated maps on the 788 distribution of rock substrates (Philibert et al., 2022; Gregr et al., 2021). Each of these products 789 was overlayed onto the final spatial predictions of sediment carbon densities and accumulation 790 rates and all cells set to zero where rock substrates were predicted. The proportional effect on the mean, upper and lower confidence interval bounds of estimates of d-carbon stock and 791 792 accumulation rates was then calculated in each bioregion.

793

794 **3. Results**

795 3.1 Mud content predictive mapping

796 Of the 25 predictor variables available for mud content random forest modelling, 13 were selected 797 in the optimal model (Fig. 3). Mean orbital velocity of waves at the seafloor and the mass of 798 suspended particulate matter at the surface were the variables with highest importance (Fig. 3). 799 Other variables with relatively high importance for predicting mud content included the exposure setting, ice thickness, distance to rivers, bathymetry, and benthic position indices (Fig. 3). Higher 800 801 mud content was generally predicted in areas of low wave velocity, low exposure and close to but 802 not directly adjacent to river mouths; with the effect of SPM and ice thickness less distinct, likely due to more complex interactive effects (Fig. 4). 803



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Figure 3. Predictor variable importance from random forest models of mud content in marine subtidal sediments. The y-axis is a unitless relative variable importance score for each model. Asterisks indicate the <u>two a</u> *priori*nitial variable predictors selection which were selected based on variable importance, with all other predictor

809 <u>variables selected using a forward selection process (see Appendix A5 for further details)</u>. WaveVel = Orbital wave
 810 velocity at the seafloor, SPM = Suspended particulate matter within the water column, BPI = Benthic position index,
 811 DistRiver = Distance to nearest river, IceThick = Sea ice thickness, Bathy = Bathymetry, VRM = Vector ruggedness

812 measure, CurrVel = Current velocity at the seafloor.







815 Figure 4. Accumulated local effects (ALE) plots for the six predictor variables with highest importance in the 816 mud content random forest model. ALE (distributions dawn by lines) gives a visual representation of the average

817 effect of the predictor variable on the response but does not indicate the influence of multi-way interactions which are

inherent in random forest models. Rug plots <u>(dashed marks at bottom)</u> indicate the distribution of each variable within
 the training dataset. SPM = suspended particulate matter.

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Areas with sediments dominated by mud (>75%) were predicted across the basins of many of the 821 822 Pacific fjords, inlets and estuaries, and within the southern Salish Sea (Fig. 5). In the Arctic, mud dominated areas included large parts of the Canadian western Arctic as well as Hudson Bay. In 823 824 the Atlantic, the Laurentian channel and central-deeper parts of the Scotian Shelf contained 825 particularly high mud fractions (Fig. 5). Across the model domain, sediment in deeper areas on the continental slope was also highly dominated by mud (Fig. 5) Using robust spatial cross 826 827 validation, the model was estimated to have an RMSE of 24.4% and R² of 0.60. The cell specific 828 upper and lower 95% CI bounds are shown in Figure D1E1. On average the upper CI bounds 829 were 28% higher larger than the mean and the lower CI bounds 20% less.



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836

838 **3.2 Organic carbon content predictive mapping**

Eleven predictor variables were selected in the optimal organic carbon content (%OC) model (Fig. 6). The variables with highest importance in predicting %OC were the mud content layers constructed above (specifically the mean and lower CI-bound), with all other predictors having less than half the relative importance of the mean mud predictions (Fig. 6). On average organic carbon content increased with predicted mud content and was generally higher in areas with low SPM concentrations, low exposure settings, close to but not directly adjacent to rivers, and at high water temperatures (Fig. 7).





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Figure 6. Predictor variable importance from random forest models for the organic carbon content in marine subtidal sediments. The y-axis is a unitless relative variable importance score. Asterisks indicate the <u>two initial</u> predictors which were selected based on variable importance, with all other predictor variables selected using a forward selection process (see Appendix A5 for further details).*a priori* variable selection. Mud_min = Lower bound of 95% CI for mud content, SPM = Suspended particulate matter within the water column, Temp = Temperature, DistRiver = Distance to nearest river, IceConc = Sea ice concentration, DO = Dissolved oxygen at the seafllor, IceThick = Sea ice thickness, CurrVel = Current velocity at the seafloor.





Figure 7. Accumulated local effects (ALE) plots for the six predictor variables with highest importance in the organic carbon (OC) content random forest model. ALE (distributions dawn by lines) gives a visual representation of the average effect of the predictor variable on the response but does not indicate the influence of multi-way interactions which are inherent in random forest models. Rug plots (dashed marks at bottom) indicate the distribution of each variable within the training dataset. SPM = suspended particulate matter.

The predictions of %OC ranged from 3×10^{-5} to 5.6% with an overall mean of 0.8 ± 0.3% (± SD). 863 Areas with highest predicted %OC (>3%) were restricted to parts of the Pacific west coast fjords 864 and channels, and in small parts of the inlets and bays on the east coast of Nova Scotia and 865 around Passamaguoddy Bay in the Bay of Fundy (Fig. 8). High concentrations (i.e. >1%) were 866 more widespread across these areas as well as covering much of the Beaufort Sea, western 867 868 Baffin Bay and Foxe Basin in the Arctic, southern and central Hudson Bay, the Laurentian 869 channel, coastal north Newfoundland and the central Scotian shelf in the Atlantic, as well as 870 across the Salish sea and deeper areas to the south of the British Colombian Pacific continental 871 margin (Fig. 8). Lowest %OC was predicted across shallower parts of the central Pacific shelf and near coast areas west of Vancouver Island (Fig. 8). Cross validation estimated an R² for the model 872 873 of 0.58 and an RMSE of 0.09 arcsin{%OC}. Cell specific upper and lower 95% CI bounds are 874 shown in Figure ED2. On average the upper CI bounds were 42% higher larger than the mean 875 prediction, and the lower CI bounds 33% less than the mean prediction.



Figure 8. Predictive mapping of organic carbon content (%) in subtidal marine sediments across the Canadian
continental margin. The main plot shows the Arctic and Atlantic regions with the Pacific region inset. The continuous
variable is shown displayed in discrete colour bands to improve visualisation of highly right skewed data. The 95%
confidence interval bounds around the predicted means are shown in Figure <u>D2E2</u>. Labels indicating the locations of
different areas mentioned within the text are shown in Figure <u>A4B3</u>. Country outlines from World Bank Official
Boundaries, available at https://datacatalog.worldbank.org/search/dataset/0038272.

883 **3.3 Sediment mass accumulation rate predictive mapping**

The optimal model for mass accumulation rate (MAR) of seabed sediments contained 10 884 885 variables (Fig. 9). On average, MAR was negatively associated with increasing ice thickness, ice 886 concentration, salinity and distance from rivers, and was particularly high in Eastern bioregions (Fig. 10). The predictions of MAR ranged from 4x10⁻⁴ to 0.35 g cm⁻² yr⁻¹ with an overall mean of 887 888 0.01 ± 0.03 g cm⁻² yr⁻¹ (± SD). Areas with highest MAR (>0.1 g cm⁻² yr⁻¹) were predicted on the 889 east coast around inshore areas of the Gulf of St Lawrence and Bay of Fundy (Fig. 11). Other 890 areas with higher than average MAR were predicted across Canadian inshore areas particularly in the southern Arctic, Hudson Bay, Foxe Basin, Salish Sea and northeast British Colombia Pacific 891 shelf (Fig. 11). The optimal model had an estimated R² of 0.89 and RMSE of 0.206 log₁₀/g cm⁻² 892 yr⁻¹}. Cell specific upper and lower 95% CI bounds are shown in Figure D3. On average the upper 893 CI bounds were 33% higher than the mean prediction, and the lower CI bounds 20% less than 894 895 their means.





910 Figure 11. Predictive mapping of sediment mass accumulation rate (g cm⁻² yr⁻¹) across the Canadian 911 continental margin. The main plot shows the Arctic and Atlantic regions with the Pacific region inset. The continuous 912 variable is shown displayed in discrete colour bands to improve visualisation of highly right skewed data. The 95% 913 confidence interval bounds around the predicted means are shown in Figure D3. Labels indicating the locations of 914 different areas mentioned within the text are shown in Figure A4. Country outlines from World Bank Official Boundaries, 915 available at <u>https://datacatalog.worldbank.org/search/dataset/0038272</u>.

917 **3.4-3 Dry bulk density estimation**

918 The dry bulk density of sediments was estimated using a variety of transfer functions and global predictions the predicted values of mud content from our random forest model, and previously 919 published functions for conversions to porosity and dry bulk density (Fig. 2). Estimated values 920 ranged from 0.67 - 1.62-61 g cm⁻³ with a mean of $1.02-04 \pm 0.216$ g cm⁻³ (± SD). As many of the 921 transfer functions are dependent on the predicted mud content, As expected by its derivation, the 922 923 spatial distribution of dry bulk density values was very similar to the mud content values predicted 924 above (Fig. 5), i.e. lowest dry bulk density was estimated in mud dominated areas (Fig. 129). Cell specific upper and lower 95% Cluncertainty bounds are shown in Figure D4E3. On average CI 925 these bounds were 8.5% either side of their means 6.2% larger and 6.0% lower than the cell-926 927 specific mean estimate.



Figure 129. Estimates of sediment dry bulk density (g cm⁻³) across the Canadian continental margin. The main
 plot shows the Arctic and Atlantic regions with the Pacific region inset. The 95% confidence intervalestimated bounds
 of uncertainty around the predicted means are shown in Figure D4E3. Labels indicating the locations of different areas
 mentioned within the text are shown in Figure A4B3. Country outlines from World Bank Official Boundaries, available
 at https://datacatalog.worldbank.org/search/dataset/0038272.

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935 **3.<u>5</u> <u>4</u> Estimated organic carbon density and standing stock**

936 From combining predictions of dry bulk density and organic carbon content, organic carbon density could be estimated across the Canadian continental margin (Fig. 2). Estimated values 937 938 ranged from 5×10^{-4} to $5 \oplus 8.04$ kg m⁻³ with a mean of 87.91 ± 2.85 kg m⁻³ (± SD). Spatial patterns in organic carbon density (Fig. 103) were similar to those found for organic carbon content (Fig. 939 8). Areas with highest carbon density (> 25 kg m⁻³) were restricted to small areas within nearshore 940 941 zones, including inlets and fjords of British Columbia (Pacific), as well as enclosed nearshore areas of the Atlantic East Coast (Fig. 103). High carbon densities (> 15 kg m⁻³) where predicted 942 to occur across wide parts of these areas as well as further offshore in parts of the Laurentian 943 channel and central Scotian Shelf, and at the edge of the continental slope off the West of 944 945 Vancouver Island (Fig. 103). In the Arctic, areas with relatively high carbon (>10 kg m⁻³) were 946 predicted across many nearshore areas, as well as across large parts of the Beaufort Shelf, Foxe 947 Basin, James Bay and the Kane Basin (Fig. 103). Cell specific upper and lower 95% Cluncertainty

bounds are shown in Figure <u>D5E4</u>. On average the upper <u>CI</u> bounds were <u>5450</u>% higher than the
 mean prediction, and the lower <u>CI</u> bounds <u>3937</u>% less than their means.

Using a standardised sediment depth of 30 cm, the total standing stock of organic carbon in surficial sediments across the model domain is estimated at 10.7–9 Gt with a 95% confidence intervaluncertainty bounds of 67.6-0 – 16.0 Gt. Between bioregions, total stock was predominantly related to the total areal extent, for example Hudson Bay having the largest carbon stock and largest area (Table 2). The Strait of Georgia and Southern Shelf bioregions of the Pacific had the lowest total standing stocks due their small extent, however per unit area, these regions contained the highest organic carbon stocks, along with the Gulf of St Lawrence.

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Figure 1310. Estimates of organic carbon density (kg m⁻³) across the Canadian continental margin. The main plot shows the Arctic and Atlantic regions with the Pacific region inset. The continuous variable is shown displayed in discrete colour bands to improve visualisation of highly right skewed data. The 95% confidence intervalestimated bounds of uncertainty around the predicted means are shown in Figure D5E4. Labels indicating the locations of different areas mentioned within the text are shown in Figure A4B3. Country outlines from World Bank Official Boundaries, available at https://datacatalog.worldbank.org/search/dataset/0038272.

966 Table 2. Summary of estimated mean total organic carbon stocks and accumulation rates in surficial seabed

967 sediments of different bioregions across the Canadian continental margin. Organic carbon standing stocks are

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estimated for the top 30 cm of seabed sediments. For delineation of the different bioregions see Supplement.

Bioregion	Model domain	OC stock	Stock per	
	extent (km ²)	(Gt)	unit area	
			(kt km²)	
1. Offshore Pacific	53,598	0. 14<u>15</u>	2. 67<u>75</u>	
2. Northern Shelf BC	96,373	0.2 <mark>3</mark> 4	2. <u>34</u> 17	
3. Southern Shelf BC	28,313	0. <u>10</u> 09	3. <u>38</u> 11	
4. Strait of Georgia	8,664	0.04	4. <u>94</u> 56	
5. Western Arctic	526,309	1. <u>09</u> 11	2. <u>06</u> 11	
6. Arctic Basin	250,178	0.4 <mark>2</mark> 5	1. <u>69</u> 78	
7. Arctic Archipelago	243,425	0.4 <u>7</u> 8	1.9 <mark>2</mark> 7	
8. Eastern Arctic	757,226	1.8 <mark>2</mark> 0	2. <u>40</u> 38	
9. Hudson Bay	1,234,257	3.0 <mark>8</mark> 3	2.4 <mark>96</mark>	
10. NL Shelves	820,462	<u>2</u> 1. <u>04</u> 95	2. <u>49</u> 38	
11. Gulf of St Lawrence	235,541	0. <u>80</u> 75	3. <u>38</u> 18	
12. Scotian Shelf	234,888	0.6 <mark>5</mark> 4	2. <u>77</u> 59	

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Notes: OC = Organic carbon; NL = Newfoundland-Labrador.

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971 3.6 Estimated organic carbon accumulation rates

972 Organic carbon accumulation rates were estimated from combining mapped products of sediment mass accumulation and organic carbon content (Fig. 2). Estimated values ranged from 3.5x10-6 973 to 76.9 g m⁻² y⁻¹ with a mean of 1.1 ± 2.8 g m⁻² y⁻¹ (± SD). The majority of the model domain was 974 estimated to have low accumulation rates with values < 0.5 g m⁻² y⁻¹ (Fig. 14). Highest 975 976 accumulation rates were restricted to the East coast of Canada across the Gulf of St Lawrence 977 and in nearshore areas of the Bay of Fundy (Fig. 14). Other areas with relatively high 978 accumulation rates were confined to near coast areas including the Salish Sea and some fjords 979 and inlets in the Pacific west coast, as well as near coast areas in Hudson Bay, Foxe Basin and the Beaufort Sea in the Arctic (Fig. 14). Cell specific upper and lower 95% CI bounds are shown 980 981 in Figure D6. On average the upper CI bounds were 88% higher than the mean prediction, and 982 the lower CI bounds 47% less than their means. Overall, the total accumulation of organic carbon across the model domain is estimated with a mean of 4.9 Mt y⁻¹ with a 95% confidence interval of 983 984 2.6 — 9.3 Mt y⁻¹. In contrast to the organic carbon standing stock, total accumulation between 985 bioregions was not strongly related to the total areal extent. The Gulf of St Lawrence was estimated to contain both the largest total annual organic carbon accumulation and the highest
accumulation per unit area (Table 2). The Strait of Georgia was estimated to have the second
highest accumulation rates per unit area, but low total carbon accumulation due to its small area
(Table 2). The Hudson Bay bioregion also included a large proportion of the organic carbon
accumulation across the model domain with the second highest total accumulation value and the
third highest mean per unit area (Table 2).



992

993 Figure 14. Estimates of organic carbon accumulation rate (g m⁻² y⁻¹) across the Canadian continental margin. 994 The main plot shows the Arctic and Atlantic regions with the Pacific region inset. The continuous variable is shown 995 displayed in discrete colour bands to improve visualisation of highly right skewed data. The 95% confidence interval 996 bounds around the predicted means are shown in Figure D6. Labels indicating the locations of different areas 997 mentioned within the text are shown in Figure A4. Country outlines from World Bank Official Boundaries, available at 998 https://datacatalog.worldbank.org/search/dataset/0038272.

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1000 **3.7-5** Rock substrate distribution case studies

As the predictive maps produced in this study rely on physical sediment samples alone, they are unlikely to produce valid estimates for areas of bedrock — i.e. estimates of zero sediment carbon density and accumulation where bedrock is located. On the Scotian shelf (bioregion 12), correcting our predictive maps with a predicted bedrock distribution map (Fig. <u>F</u>=1) reduces total organic carbon stock estimates in this region by between 7.5-7 – 7.68% leading to a value of 0.56 59 Gt (95% CI 0.33-37 – 0.87 90 Gt), and reducing total accumulation by 12.7 - 15.9% to a total of 0.18 Mt y⁻¹ (95% CI 0.08 – 0.44 Mt y⁻¹). For the Pacific British Columbian marine region (bioregions 1-4), assigning zero values to areas covered by a predicted bedrock distribution map (Fig. E2F2) would reduce our estimates by 89.51 – 9.70% to a total of 0.44 46 Gt (95% CI 0.26 29 – 0.7169 Gt) for of organic carbon stock and reducing by 13.8 – 15.3% to a total of 0.08 Mt y⁻¹ 1011 ¹ (95% CI 0.03 – 0.23 Mt y⁻¹) for organic carbon accumulation.

1012

1013 4. Code and data availability

1014 All mapped products as shown in Figures 5, 8, 11, 129, and 10, 3 and 14 have been made available 1015 TIFF georeferenced files in the Borealis data repository as at 1016 https://borealisdata.ca/privateurl.xhtml?token=7bb00f1e-2ce3-400c-955d-e8e0d4fe3080 1017 (Epstein et al., 2023). This includes the mean predictions as well as the cell-specific 1018 95% uncertainty confidence interval bounds as shown in Appendix DE. The repository also 1019 contains all data collated within the systematic data review of organic carbon content and the 1020 georeferenced TIFF files from the rock distribution case studies (Appendix EF). Additionally, all 1021 the associated code used for data manipulations, model building and predictive mapping can also 1022 be found within the above repository.

1023

1024 **5. Discussion**

1025 Using best available data, we have produced the first national assessment of organic carbon in 1026 surficial seabed sediments across the Canadian continental margin, estimating the standing stock 1027 in the top 30 cm to be 10.7-9 Gt (95% CI 67.06 – 16.0 Gt). Although comparisons to previous 1028 global studies is challenging due to differences in sediment reference depths, mapping resolutions 1029 and total spatial coverage, our estimate falls within a similar range to those previously published (e.g. 2.2 Gt in the top 5 cm (Lee et al., 2019) and 48 Gt in the top meter (Atwood et al., 2020) of 1030 1031 the Canadian EEZ). In contrast to these global studies, the national approach taken here allows 1032 for a more complete data synthesis, a finer spatial resolution, larger spatial coverage of the 1033 Canadian continental margin and spatially explicit defined estimates of uncertainty; all of which allow for higher confidence in the predictive mapping products and overall estimates of standing 1034 1035 stock. Similarly to other national and regional mapping studies (Smeaton et al., 2021; Diesing et al., 2017, 2021), areas of high organic carbon stocks were predominantly predicted to occur in
coastal fjords, inlets, estuaries, enclosed bays and sheltered basins, as well as in deeper
channels and throughs troughs (Fig. 103). To put our estimated organic carbon standing stock
into context, 10.7–9 Gt equates to 5152% of the organic carbon estimated to be stored in all
Canadian terrestrial plant live biomass and detritus (both above and below ground), and 349.8%
of soil organic carbon to 30 cm across Canada (assuming equal distribution of soil carbon in the
top 1 m) (Sothe et al., 2022).

1043 Due to a lack of available data, we were unable to undertake a fully independent predictive 1044 mapping exercise for organic carbon accumulation rates on Canadian seabed sediments. However, our downscaling exercise of a recently published global product on mass accumulation 1045 1046 rates, coupled with the national predictive mapping of sediment organic carbon content, led to an 1047 estimated annual accumulation at the seafloor of 4.9 Mt of organic carbon per year (95% CI 2.6 -9.3 Mt y⁻¹). Given the extent of the model domain (~1.25% of the global ocean), this estimate 1048 1049 again falls close to the range of previous global predictions - i.e. 1.25% of global accumulation at 126-350 Mt y⁻¹ is 1.6-4.4 Mt y⁻¹ (Keil, 2017; Berner, 1982). Areas of high accumulation were 1050 1051 predominantly restricted to the Gulf of St Lawrence and Bay of Fundy, as well as other near-coast 1052 areas where large river outlets co-occurred with predicted areas of high carbon density (Fig. 10, 1053 13, Supplement).

1054

1055 Model interpretation and uncertainties

1056 The two key components of the carbon stock estimates in this study are the predictive maps for 1057 mud content and organic carbon content, which were estimated to have a map accuracy of 60% and 58% respectively (R² 0.60 and 0.58). While these values may seem relatively low when 1058 1059 compared to some other related studies (Diesing et al., 2017, 2021; Atwood et al., 2020; Mitchell 1060 et al., 2019), the use of robust, spatially explicit cross-validation to calculate model evaluation 1061 metrics (as we did herein) has been shown to produce significantly more conservative estimates 1062 of map accuracy when compared to frequently used random cross-validation approaches (Ludwig 1063 et al., 2023; Meyer et al., 2019) such as those used in both the global seabed carbon stock studies 1064 discussed above (Atwood et al., 2020; Lee et al., 2019). Within this study, we also calculated cell 1065 specific confidence intervaluncertainty bounds to give spatially explicit estimates of uncertainty. While there are many ways to calculate model uncertainty, therefore making comparisons 1066 1067 between studies challenging, the uncertainty in carbon density calculated here (CI-3937-5450%

either side of the mean) is close to those found within similar regional (Diesing et al., 2021; 58%)
and global studies (Lee et al., 2019; 49%), both of which predict carbon stocks at significantly
coarser resolutions. Our 95% confidence interval bounds for total standing stock (3836% lower
and 5047% higher than the mean) are also similar to the estimated bounds from the recently
published predictive models of Canadian terrestrial vegetation and soil carbon (a 90% confidence
interval 48% either side of the mean) (Sothe et al., 2022).

1074 Higher map accuracy was estimated for mass accumulation rate (R² 0.89); however, it is important 1075 to recognise that this only describes the accuracy of our downscaled product to represent the global spatial product from which data were sampled. This global model was itself estimated to 1076 1077 have an R² of 0.88 for empirical point data, however this was calculated with traditional random 1078 cross-validation techniques (Restreppo et al., 2021). The estimated values of organic carbon 1079 accumulation rate predicted here should be used with some caution as there is likely significant 1080 uncertainty that is not truly quantified due to the small amount of in-situ empirical data from the 1081 Canadian continental margin (Restreppo et al., 2021). The mean confidence interval for organic 1082 carbon accumulation estimated in this study was also very wide at its upper bound (88% above 1083 mean). This is largely due to the highly right skewed distribution of predictions, with a 1084 preponderance of small accumulation rate values, meaning a small absolute increase in 1085 estimated accumulation can have very large proportional effects when compared to the mean. 1086 Even so, the estimates of organic carbon accumulation made here give our current best estimate for the Canadian continental margin, and while the absolute values may contain high uncertainty, 1087 the spatial patterns between areas across the model domain are expected to have higher 1088 1089 confidence.

1090 Using two case studies from British Columbia and the Scotian Shelf, we estimated that the 1091 distribution of rock substrates could reduce our estimates of carbon stock by approximately 7.5-7 1092 -_ 9.07% and carbon accumulation by 12.7 - 15.3% (Fig. E1F1, E2F2). As much of the Canadian 1093 coastline is distant from significant infrastructure, extensive surveys of the seafloor are generally 1094 lacking, especially when compared to similar regional carbon mapping studies in northwest 1095 Europe (e.g. Smeaton et al., 2021). It is therefore unclear how representative these case studies 1096 are of the entire Canadian EEZ. Improved data on the presence of bedrock across lesser studied 1097 regions of the Canadian Arctic, Hudson Bay, Gulf of St Lawrence, Newfoundland and Labrador 1098 may allow for the production of a predictive map of bedrock across the Canadian EEZ which 1099 would significantly improve the carbon estimates and spatial predictive maps produced in this 1100 study.

1101 Areas of uncertainty which could not be fully quantified include the accuracy and precision of 1102 response data and predictor layers. The response data drive the model construction, and 1103 therefore sampling, processing, or recording errors can propagate into predictions. This is 1104 particularly relevant given the large temporal extent of response data which was required to gain 1105 sufficient coverage for this work (1959-2019). This large duration may also add additional variation from temporal differences between data, for example from differing anthropogenic drivers on 1106 1107 carbon storage and/or accumulation (Keil, 2017); however, similar temporal extents have been used in related studies (Atwood et al., 2020; Lee et al., 2019; Seiter et al., 2004) and 72% of the 1108 1109 organic carbon data within this study were sampled after 1980 and 55% after 2000. Within the 1110 response data, assumptions and/or predictions were also required regarding the distribution of mud and carbon across sediment depths. While standardising for this factor is clearly necessary, 1111 1112 especially when using a wide variety of legacy data, it does add additional uncertainty which would not be present if widescale standardised sampling methods were employed. The results from this 1113 1114 study do however highlight, that within the top 30 cm of sediment, the spatial location of the sample is a far stronger driver of organic carbon content than the sediment sampling depth (Table 1115 1116 <u>B1C1</u>).

1117 Most of the predictor variables used in this study are also themselves modelled products, which 1118 contain their own inherent uncertainties and/or interpolations which cannot be fully quantified 1119 here. Additionally, many predictors are constructed at spatial resolutions significantly coarser than 1120 that used for modelling and prediction in this study. This meant that predictor data had to be interpolated, with significant inherent assumptions regarding variation and distribution of the data. 1121 Although best available data were used in this study, if predictor variables were available at higher 1122 1123 native resolutions, less assumptions would be necessary and significant differences may be found in predictions, as well as their uncertainty and variability. mMany of the predictor variables also 1124 1125 have temporal components, and while the climatological mean of a 12 - 14 year timespan used 1126 in this study is expected to produce variables representative for the study region, they do not 1127 completely align with the temporal extent of the response data which could add further prediction 1128 uncertainty. Finally, due to data availability, the uncertainty bounds around our mean estimates of dry bulk density and organic carbon density were approximated from the constructed 95% CIs 1129 1130 of mud content and %OC from the random forest models. While these provide an appropriate measure of uncertainty in our estimates in the context of this study, if large empirical datasets 1131 1132 became available for dry bulk and organic carbon density, it would be preferable to construct 1133 predictive models, mean estimates and uncertainty bounds for these response variables directly.

1135 Future directions and applications

1136 Improvements could be made in future iterations of these sediment carbon maps when additional response data become available. The size of the organic carbon content dataset was relatively 1137 1138 small (2,518 point-samples) given the size of the model domain, so new data could greatly 1139 improve accuracy and reduce uncertainty in predictions. Additionally, wide-spread in-situ 1140 empirical data on sediment dry bulk density and sediment mass accumulation rates would reduce 1141 the assumptions needed in using transfer approximate conversions from mud content, functions 1142 and downscaling models; however, large datasets would be needed to conduct robust 1143 independent modelling exercises. while a large geographically dispersed empirical dataset on 1144 seabed sediment organic carbon density (i.e. where OC content and dry bulk density is measured 1145 directly in each physical sample) would reduce assumptions even further, with the potential to 1146 construct a single predictive map for this response alone (Diesing et al., 2021). -There are also 1147 improvements to be made with the development of higher resolution or more accurate predictor 1148 layers. This would be particularly relevant for those variables with coarse resolutions and those 1149 which were seen to have highest importance within our models or from related seabed sediment 1150 mapping studies (e.g. Gregr et al., 2021; Diesing et al., 2017, 2021; Mitchell et al., 2019) - i.e. 1151 wave velocities, suspended particulate matter, exposure, current velocities and oxygen 1152 concentrations. Further validation and refinements could also be supported by numerical 1153 biogeochemical modelling products where the organic carbon densities and/or accumulations are mathematically estimated based on oceanographic, climatological and benthic conditions, 1154 1155 including the potential to incorporate predictions under different future climate scenarios (Ani and 1156 Robson, 2021).

1157 The organic carbon predictive mapping products generated here could have many future applications. Regionalisation and prioritisation processes could identify key areas of carbon 1158 storage for further research and possible protections (Epstein and Roberts, 2022, 2023; Diesing 1159 1160 et al., 2021). There is also potential to combine these mapped products with spatial data on 1161 human activities occurring on the seafloor to consider potential management implications, such 1162 as controlling the levels of impactful industries (e.g. mobile bottom fishing, mineral extraction, 1163 energy generation) in areas with high organic carbon storage/accumulation areas (Clare et al., 1164 2023; Epstein and Roberts, 2022). The mud content predictive maps may also have applications 1165 for marine planning more widely, being a strong driver of the biological habitat type and sensitivity. 1166 Overall, these data have wide-scale relevance across marine ecology, geology and environmental management disciplines, however, the use of these products should always consider the
 discussed uncertainties and quantified confidence interval<u>uncertainty</u> bounds of predictions. As
 with all large-scale mapping exercises, continued *in-situ* empirical data collection is needed for
 improved accuracy of mapping seabed carbon stocks and accumulation rates across Canada.

1171 6. Appendices

1172 Appendix A. Supplementary methods

1173 <u>2.A1. Analysis software</u>

1174 Analyses were primarily undertaken in R 4.2.2 (R Core Team, 2022) and Rstudio 2022.12.0.353 1175 (Posit Team, 2022), with some additional data manipulation and spatial plotting in QGIS 1176 (QGIS.org, 2021) and Python (Van Rossum and Drake, 2009). Within R, raster data were handled using the terra package (Hijmans, 2022), spatial vector data using the sf package (Pebesma, 1177 1178 2018), netCDF data with the stars (Pebesma, 2022) and tidync (Sumner, 2022) packages, data-1179 frames with the dplvr package (Wickham et al., 2019), and vector data with base R (R Core Team, 2022). Random forest modelling was primarily dependent on the ranger package (Wright and 1180 1181 Ziegler, 2017), however models were constructed and tuned using the *tidymodels* package (Kuhn 1182 and Wickham, 2020), with cross-validation and predictor variable selection using the CAST (Meyer et al., 2023) and caret (Kuhn, 2022) packages. Plotting utilised the above packages as 1183 1184 well as gaplot2 (Wickham et al., 2019) and patchwork (Pedersen, 2022) while parallel processing 1185 used the *doParallel* package (Microsoft Corporation and Weston, 2022).

1186

1187 A2. Bathymetry layer construction

1188 To define the maximum potential spatial coverage of this study, best available bathymetric datasets were combined across the Canadian Exclusive Economic Zone (EEZ) (Table 1). Firstly, 1189 1190 three Digital Elevation Model (DEM) raster layers covering different extents of the Canadian EEZ were each filtered to contain only those elevations of less than or equal to 0 m. Where necessary, 1191 1192 data were then aggregated (averaged) or disaggregated (split) to a resolution of approximately 1193 200 m, and all layers were projected onto a unified 200 m x 200 m equal area grid (co-ordinate 1194 reference system (CRS) EPSG:3573 -- WGS 84 -- North Pole Lambert Azimuthal Equal Area 1195 Canada). Reprojection was necessary as all three DEMs were in different co-ordinate systems. including some already being projected. The 200 m resolution was chosen as it is the median 1196 1197 native resolution of the three DEMs, while also being considered towards the upper limit of what 1198 may be computationally possible within the scope of this study. After reprojection, the three layers 1199 were overlain, with the region-specific data given priority over global data where present. Finally, 1200 the seaward boundaries were delineated by the outer extent of the Canadian EEZ (Flanders 1201 Marine Institute, 2019).

1202 1203 A3. Details of ocean circulation models 1204 ANHA12 is a regional configuration of the NEMO ocean and sea-ice model (Madec et al., 1998) 1205 created at the University of Alberta, covering the Arctic and northern Hemisphere Atlantic at 5 day temporal resolution, a curvilinear 1/12th degree horizontal resolution ranging from 1.93 km in the 1206 1207 Arctic to 9.3 km at the equator, and 50 vertical levels (Hu et al., 2019). The British Columbia continental margin (BCCM) circulation model created by Fisheries and Oceans Canada (DFO) 1208 1209 covers the entire Canadian Pacific coast and extends approximately 400 km offshore. It has a 1210 uniform horizontal resolution of 3 km, 42 vertical levels and a 3 day temporal resolution (Peña et al., 2019; Masson and Fine, 2012). As the BCCM model has higher uncertainty in nearshore and 1211 1212 enclosed environments due to its relatively coarse resolution, data waswere also extracted for the 1213 enclosed Salish Sea from the Salish Sea Cast ERDDAP data server. Similarly to the ANHA12 1214 model, the Salish Sea Cast is a configuration of the NEMO circulation model developed by a 1215 consortium of Canadian Universities and government agencies and extends from Juan de Fuca 1216 Strait to Puget Sound to Johnstone Strait at 500 m horizontal resolution, 40 vertical lavers and 1217 hourly temporal resolution (Soontiens and Allen, 2017; Soontiens et al., 2016). For further details 1218 on all these models, see relevant cited references. It should be noted that many of these ocean 1219 circulation models contain high uncertainty in nearshore areas. However, they are expected to be 1220 greatly improved when compared to global circulation model products (Peña et al., 2019; Hu et 1221 al., 2019; Soontiens and Allen, 2017) which are frequently used in this sort of predictive mapping 1222 work (e.g. Atwood et al., 2020; Lee et al., 2019; Assis et al., 2018). 1223

1224 A4. Sediment grain size data collation and processing details

1225 Sediment composition point data were extracted from two sources. Firstly, all data were exported 1226 from the NRCan Expedition Database on 11th November 2022. This data repository contains 1227 information related to marine and coastal field surveys conducted by or on behalf of the Geological 1228 Survey of Canada from the 1950s to present, which deployed sampling methods including piston cores and grab samples. Data were also extracted from a recent synthesis of grain size 1229 1230 distribution measurements from the Canadian Pacific seafloor (1951-2017), compiled by Geological Survey Of Canada and NRCan (Enkin, 2023). Although there are some duplications 1231 between these two datasets, these are accounted for in the proceeding pre-processing steps. In 1232 both sources, grain size data is reported as the percentage content of mud (sometimes separated 1233

1234 into silt and clay), sand and gravel within each sample. Due to modern developments in grain size 1235 analyses (e.g. laser diffraction) older samples may have lower measurement accuracy; however, due to the relatively coarse metric being used in this study (%mud/sand/gravel) and the 1236 1237 occurrence of a number of largescale geological surveys occurring during the 1960s, we chose 1238 to retain data from 1960 onwards. Where sampling year was not recorded within the database. 1239 the date was inferred from the expedition code or from expedition metadata. The sampling method 1240 and depth of the sediment from which the sample/sub-sample originates are also predominantly 1241 recorded within the database. Where sediment depth was absent, but the sampling method was 1242 noted as "grab" or "other", the penetration depth was assumed to be 10 cm (a commonly assumed 1243 penetration of standard sediment sampling devices such as Van Veen Grabs and Day Grabs). 1244

1245 A5. Details on construction and implementation of spatial cross validation and feature selection

1246 For each response variable modelled in this study (mud content and organic carbon content 1247 (%OC)), the spatialsample package (Silge and Mahoney, 2023) was used to construct a variety 1248 of spatial CV data-fold structures and the validity of each structure was visually assessed using 1249 the CAST.plot geodist function (Meyer et al., 2023). This function creates density plots of nearest 1250 neighbour distances (Euclidean) in multivariate predictor space (using normalized variables) 1251 between response data locations and a random sample of prediction locations, and between data 1252 inside and outside each CV fold (Ludwig et al., 2023; Meyer et al., 2023; Meyer and Pebesma, 1253 2022). The suitability of a given CV structure to be representative of estimating map accuracy can 1254 be determined by visually assessing the density plots and finding the CV-distance curve being 1255 closely aligned to the density curve of response data to prediction distances (see Appendix D; 1256 Ludwig et al., 2023; Meyer and Pebesma, 2022). To approximate response-to-prediction 1257 distances, the sample size number within plot_geodist was set to select 5,000 random samples 1258 across the model domain. Further, as the spatial distribution of data is a key consideration to 1259 ensure robust cross-validation (Ludwig et al., 2023; Meyer and Pebesma, 2022), for the 1260 plot_geodist calculations alone, the x- and y-coordinates of each data point were included in 1261 addition to those predictor variables listed in Table 1 and described in Section 2.5.

For the mud content data, a spatial kmeans clustering CV structure was chosen as the response
 data had good coverage of the model domain, contained a large number of data points, and
 showed relatively strong spatial clustering (Fig. B1). A range of options in the number of kmeans
 clusters were tested, with 35 being determined as the optimal number and each cluster being

1266 assigned to its own CV fold (Fig. D1). Through visual assessment of the density plots, it was 1267 identified that the kmeans CV structure was somewhat mis-aligned from response-to-prediction 1268 distances, with the CV distances being overly conservative at including near-distance comparisons (Fig. D1). We therefore used a partially repeated CV strategy, with a small number 1269 of randomly selected data-points added to the assessment set in each kmeans spatial-CV fold 1270 1271 (1% of mud content data randomly sampled at each fold without replacement) (Fig. D2). As the 1272 %OC response dataset was relatively small and spatially dispersed (Fig. B2), we used a spatial 1273 block CV strategy in place of the kmeans clustering to avoid clusters containing highly spatially 1274 dispersed data. We chose to use hexagonal shaped blocks, random assignment of blocks to folds, 1275 and the same number of CV folds as for the mud content data (v = 35) – both to maintain 1276 uniformity and because varying the fold-number did not significantly influence the density plots. 1277 Instead, the diameter of the spatial blocks was altered, and an optimal block size of 100 km identified using the plot geodist function (Fig. D3). 1278

1279 The CAST.ffs function (Meyer et al., 2023) was used to run a forward predictor variable selection 1280 process with appropriate spatial considerations. The function fits a model with all combinations of 1281 two-way predictors, selects the best model based on a given metric, and then increases the 1282 number of predictors by one, testing all remaining variables. This iteratively continues with the process stopping if none of the tested variables increases the performance when compared to 1283 1284 the best previous model with "n-1" predictors. The function also allows models to be fit separately 1285 across all individual on each spatial CV fold (as defined above), s, with the overall performance of each iteration based on model accuracy across all CV folds. This therefore 1286 1287 incorporatingincorporates appropriate spatial considerations into the feature selection process. Due to the large number of variables within this study, and the relatively large datasets, this 1288 1289 process was very computationally expensive. We therefore chose to adapt the function to initiate 1290 forward variable selection after a priori initial identification of the first two predictor variables. These 1291 variables were identified by constructing a basic single random forest model with all training data 1292 and predictor variables, and the hyperparameters mtry (the number of variables to randomly 1293 sample as candidates at each split), min n (the number of observations needed to keep splitting 1294 nodes) and trees (the number of random forest trees to construct and take mean predictions 1295 across) set to 2, 5 and 1,000 respectively. Variable importance was estimated on out-of-bag 1296 samples using permutation through permutation of predictor variable values (Wright et al., 2016), 1297 and the two predictor variables with largest highest importance selected. The ffs function was then 1298 run starting with the two pre-selected variables (see Fig. 3 $\&_{T}$ 6-&-9) and performance of each 1299 iteration assessed on the root mean squared error (RMSE) of predictions across all CV folds.

13001301Appendix AB. Distribution of response data





1303 Figure A1<u>B1</u>. Map showing the distribution of mud content samples across the model domain.

1304



1306 Figure A2B2. Map showing the distribution of carbon content samples across the model domain.





Hudson Bay

250

0

90°W

Gulf of St Lawrence

& Laurentian Channel

> Pass Bay

James

Bay

500 750 1,000 km

1314 The locations are for guidance only and do not represent the entire extent or exact location of a given area. Country

1315 outlines are derived from World Bank Official Boundaries, available at

1316 <u>https://datacatalog.worldbank.org/search/dataset/0038272</u>.

BC

Pacific

45°N

1310

F British

Columbia

120°W

Salish Sea

60°W

1317
1318
1319
1320 Appendix <u>BC</u>. Organic carbon sediment depth modelling results

There was a significant effect of sampling depth on the organic carbon content in seabed sediments ($\chi^2 = 1400.9$, p < 0.001). While sample ID explained most of the variation between sub-sample carbon contents, the sampling depth was also a significant factor (Table B1<u>C1</u>). Carbon content decreased with increasing sampling depth (Fig. B1<u>C1</u>). The rate of carbon content decline generally decreased with increasing depth into the sediment, however uncertainty in this trend increased within deeper sediment layers (Fig. B1<u>C1</u>).

- 1327
- 1328

1329Table B4C1. Results from the generalised additive mixed model between the carbon content of marine1330sediments and sampling depth. A basic generalised additive mixed model with a scaled-t distribution was constructed1331for carbon content in sediment sub-samples with sample ID as the random factor and sampling depth as the fixed1332factor.

Spline	Туре	edf	Res. df	X ²	Deviance explained	р
Sampling depth (cm)	Cubic	4.28	5.36	2299	1.1%	< 0.001
ID	Random	181.94	182.00	715046	86.9%	< 0.001

1333 Notes: edf = Effective degrees of freedom. Res. df = Residual degrees of freedom

1334



Figure **B4<u>C1</u>**. Regression splines indicating the effect of sediment sampling depth (a) and sample ID (b) on the organic carbon content in seabed sediment sub-samples.

The predicted mean effect of sediment depth on carbon content was extracted from the model and converted into a transfer function which states the expected ratio between the <u>cumulative</u> carbon content <u>at across</u> 30 cm compared to <u>the cumulative mean at</u> any given sampling depth (Figure <u>B2C2</u>). The ratio ranged from 89.3% when only measuring the sediment surface, to 93.7% if measuring the carbon content across the top 10 cm, and by 25 cm was approaching equilibrium at 98.8%.

1345



1346

1347 Figure **B2<u>C2</u>**. Transfer function for cumulative mean organic carbon (OC) content at 30 cm sediment depth.

Using a generalised additive mixed model an estimated transfer function was constructed to standardise the cumulativemean carbon content at any given depth to an expected value at 30 cm.

1350

1351 Appendix <u>CD</u>. Results from random forest cross-validation structure selection



1353Figure C4D1. Multivariate nearest-neighbour distance density plot for mud content data with the optimal1354number of spatial k-means clusters across cross validation (CV) folds. Frequency of nearest neighbour distances1355(x-axis) is shown for sample-to-sample distance (red), sample-to-prediction distance (green) and CV fold analysis-to-1356assessment distance (blue). dist = Multivariate Euclidean distance in predictor space after normalization of predictors.1357An optimal number of 35 clusters was selected to due close overlap between the CV-distance and sample-to-prediction1358curve.



1360Figure C2D2. Multivariate nearest-neighbour distance density plot for mud content data with a partially1361repeated spatial-random mixture method for cross validation (CV) folds. Frequency of nearest neighbour1362distances (x-axis) is shown for sample-to-sample distance (red), sample-to-prediction distance (green) and CV fold1363analysis-to-assessment distance (blue). dist = Multivariate Euclidean distance in predictor space after normalization of1364predictors. Due to the optimal spatial k-means clustering showing poor overlap at lower multivariate distances (Fig.1365C4D1), a 1% random sample without replacement was added to each fold.



1368Figure C3D3. Multivariate nearest neighbour distance density plot for organic carbon content data with the1369optimal block size across cross validation (CV) folds. Frequency of nearest neighbour distances (x-axis) is shown1370for sample-to-sample distance (red), sample-to-prediction distance (green) and CV fold analysis-to-assessment1371distance (blue). dist = Multivariate Euclidean distance in predictor space after normalization of predictors. An optimal1372block size of 100 km was selected to due close overlap between the CV-distance and sample-to-prediction curve.



Figure C4. Multivariate nearest neighbour density plot for sediment mass accumulation rate data. Frequency of
 nearest neighbour distances (x-axis) is shown for sample to sample distance (red) and sample to prediction distance
 (green). The close overlap indicates that random cross-validation will produce valid results.

1378 Appendix <u>**PE</u>**. Cell-specific <u>confidence intervaluncertainty</u> bounds for predictive sediment</u>

1379 maps



1380

1381 Figure **D1**<u>E1</u>. Estimated lower (a) and upper (b) bounds of the 95% confidence interval for predictions of mud

- content (%) in subtidal marine sediments across the Canadian continental margin. Within each panel the main
 plot shows the Arctic and Atlantic regions with the Pacific region inset.
- 1383 plot shows the Arctic and Atlantic regions with the Pacific region

1384



1385

1386Figure D2E2. Estimated lower (a) and upper (b) bounds of the 95% confidence interval for predictions of carbon1387content (%) in subtidal marine sediments across the Canadian continental margin. The continuous variable is1388shown in discrete colour bands to improve visualisation of highly right skewed data. Within each panel the main plot1389shows the Arctic and Atlantic regions with the Pacific region inset.



1392Figure D3. Estimated lower (a) and upper (b) bounds of the 95% confidence interval for predictions of mass1393accumulation rate (g cm⁻² yr⁻¹) on subtidal marine sediments across the Canadian continental margin. The1394continuous variable is shown in discrete colour bands to improve visualisation of highly right skewed data. Within each1395panel the main plot shows the Arctic and Atlantic regions with the Pacific region inset.



1397

1398Figure D4E3. Estimated lower (a) and upper (b) <u>uncertainty</u> bounds <u>aroundof</u> the <u>95% confidence interval for</u>1399mean predictions of dry bulk density (g cm⁻³) of subtidal marine sediments across the Canadian continental

1400 margin. Within each panel the main plot shows the Arctic and Atlantic regions with the Pacific region inset.





1403Figure D5E4. Estimated lower (a) and upper (b) uncertainty bounds of around the 95% confidence interval for1404mean_predictions of organic carbon density (kg m⁻³) in subtidal marine sediments across the Canadian1405continental margin. The continuous variable is shown in discrete colour bands to improve visualisation of highly right1406skewed data. Within each panel the main plot shows the Arctic and Atlantic regions with the Pacific region inset.



Figure D6. Estimated lower (a) and upper (b) bounds of the 95% confidence interval for predictions of organic
 carbon accumulation rates (g m⁻² y⁻¹) on subtidal marine sediments across the Canadian continental margin.
 The continuous variable is shown in discrete colour bands to improve visualisation of highly right skewed data. Within
 each panel the main plot shows the Arctic and Atlantic regions with the Pacific region inset.

1415 Appendix EF. Bedrock distribution case studies



1416

- 1417 Figure E1F1. Predicted mean values of organic carbon density and accumulation rates within the Scotian Shelf
- 1418 overlayed by the estimated distribution of rock substrates. Data on the estimated distribution of rock on the
- 1419 seafloor across the Scotian Shelf Bioregion is taken from Philibert et al. (2022).
- 1420

1421



1423Figure E2F2. Predicted mean values of organic carbon density and accumulation rates within the British1424Columbia EEZ overlayed by the estimated distribution of rock substrates. Data on the estimated distribution of

1426 **7. Author contributions**

JKB and SDF secured funding and led the management of this project. GE, SDF and JKB
conceptualised this study. GE, DH, AP, CP & PGM collated the data. GE developed the model
code and performed the investigations with input from SDF and JKB throughout. GE prepared the
manuscript with contributions from all co-authors.

1431

1432 8. Competing interests

1433 The authors declare that they have no conflict of interest.

1434

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1447

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