

1 Evidence for carbonate system mediated shape shift in intertidal
2 predatory gastropod

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9 Abstract

10 Phenotypic plasticity represents an important first-line organism response to newly introduced or changing
11 environmental constraints. Knowledge about structural responses to environmental stressors could thus be
12 an essential measure to predict species and ecosystem responses to a world in change. In this study, we
13 combined morphometric analyses with environmental modelling to identify direct shape responses of the
14 predatory gastropod *Nucella lapillus* to large-scale variability in sea surface temperature and the carbonate
15 system. Our models suggest that the state of the carbonate system and, more specifically, the substrate
16 inhibitor ratio ($[HCO_3^-][H^+]^{-1}$) (SIR) has a dominant effect on the shell shape of this intertidal muricid.
17 Populations in regions with a lower SIR tend to form narrower shells with a higher spire to body whorl ratio,
18 whereas populations in areas with a higher SIR form wider shells with a much lower spire to body whorl ratio.
19 These results indicate that a widespread phenotypic response of *N. lapillus* to continuing ocean acidification
20 can be expected, potentially altering the phenotypic response pattern to predator or wave exposure regimes
21 with profound implications for North Atlantic rocky shore communities.

22 **Keywords:** biomineralisation, resistance, shape plasticity, calcification, compensatory mechanisms, multiple
23 stressors, climate change, dog whelk, Thais, ocean acidification

24 Introduction

25 Together with genetic predispositions, environmental constraints are the primary causes for shape variability
26 within and among populations. Phenotypic plasticity is the ability of a single genotype to produce a range of
27 different forms in response to its environment.¹⁻³ This trait, if adaptive, is generally perceived advantageous
28 for an organism or population because it facilitates resistance to a range of different stressors allowing
29 similar genotypes to populate heterogeneous habitats.⁴ Therefore, changes in morphology can be strong
30 indicators for increasing or changing environmental stressors, knowledge about which may be important
31 when monitoring the consequences of anthropogenically induced global climate change.⁵ So far, studies have
32 focused predominately on population and community composition responses⁶ or genetic markers to study
33 the effect of global change. However, an understanding of phenotypic consequences was also found to be
34 crucial to forming a complete picture of biological responses to a world in change.^{5,7-10}

35 Climate change associated with rising atmospheric carbon dioxide levels, increasing terrestrial and seawater
36 temperatures, ocean acidification (OA) and more frequent extreme weather events is an emerging global
37 threat to most of the Earth's biosphere.¹¹ In the oceans, annually increasing sea surface temperatures and
38 OA pose strong stressors for marine organisms.^{12,13} Species with calcium carbonate ($CaCO_3$) shells or

39 skeletons are expected to be especially impacted by global climate change.^{14–18} The reduction in seawater
 40 pH associated with rising atmospheric CO_2 concentration results in potentially harmful effects (e.g., shell
 41 dissolution), making an organism more susceptible to predation, parasites, or infectious diseases.^{19–21} Marine
 42 calcifiers are reported to be especially vulnerable at the larval stage to the synergistic effects of OA and ocean
 43 warming,¹⁴ as this can lead to premature death or severe retardation of shell formation.^{16,22,23} To overcome
 44 these impacts, $CaCO_3$ bearing organisms are required to spend a larger proportion of their metabolic energy
 45 on calcification to maintain the *status quo*,²⁴ which could have far-reaching implications for their energy
 46 balance and competitiveness.

47 There is a consensus that calcification is linked to $CaCO_3$ substrate abundance and speciation, i.e., to
 48 the $CaCO_3$ saturation state Ω_{CaCO_3} in seawater, although its exact role in the acidified ocean is still
 49 debated.^{25–27} The Ω_{CaCO_3} is a function of both calcium ion $[Ca^{2+}]$ and bicarbonate $[CO_3^{2-}]$ availability as
 50 well as the thermodynamic solubility product K_{sp} of the respective $CaCO_3$ polymorphs (for molluscs, most
 51 important are aragonite and calcite) at a specific pressure, salinity and temperature²⁸ (eq. 1).

$$\Omega_{CaCO_3} = \frac{[Ca^{2+}][CO_3^{2-}]}{K_{sp}} \quad (1)$$

52 In seawater, both $[Ca^{2+}]$ and the dissolved inorganic carbon concentrations (DIC) are tightly coupled to
 53 seawater salinity, whereby the speciation of DIC in seawater is pH-dependent. This means that both a
 54 reduction in the salinity and the pH can reduce the saturation state of seawater. At $\Omega_{CaCO_3} < 1$, $CaCO_3$
 55 dissolution becomes thermodynamically favourable; however, as pointed out by Waldbusser et al. (2016),
 56 low Ω_{CaCO_3} states likely pose more of a kinetic rather than a thermodynamic constraint on marine calcifiers
 57 considering the rapid rate of calcification observed especially at the larval stage.²⁵ Irrespective of whether
 58 thermodynamic or kinetic bottlenecks are responsible, continuously low Ω_{CaCO_3} states can have serious
 59 implications for shell-forming organisms.^{17,29,30} In recent years, many *in-situ* and laboratory studies have
 60 added to our understanding of the effect of climate change on marine calcifiers.^{9,12,13,31–34} However, rela-
 61 tively short-term experiments,³⁵ heterogeneous study designs, and partly conflicting results among studies
 62 have complicated interpretations and highlight the complexity of possible organism responses to a changing
 63 environment. While long-term, multi-generational experiments are key to studying phenotypic and genetic
 64 adaptations to environmental change,³⁵ they require many months to years and thus pose a serious time
 65 constraint.^{36,37} This is especially true if organisms with long lifespans and/or a slow reproductive cycle are
 66 to be studied. Thus different approaches to investigating the effect of climate change in a natural setting
 67 that also account for both phenotypic and genetic adaptations receive increasingly more attention.^{8,9,38,39}

68 These kind of studies focus on organism responses in the temporal domain by comparing archival collections
69 with modern specimens collected from a strongly constrained spatial range^{8,9,40} or in the spatial domain by
70 studying the effect of environmental constraints on an organism over an extensive geospatial range, made
71 possible by recent advancements in ecological modelling.^{5,38}

72 The dog whelk, *Nucella lapillus* (Linnaeus, 1758), is an important predatory gastropod inhabiting the rocky
73 intertidal zone of the North Atlantic.^{41,42} *Nucella lapillus* preys predominately on habitat-forming founda-
74 tion species such as blue mussels or barnacles and thereby exerts a strong top-down control on rocky-shore
75 ecosystems.⁴³⁻⁴⁵ Its spatial distribution ranges from the northern tip of Norway to southern Portugal, span-
76 ning three climate zones. *Nucella lapillus* is a direct-developing gastropod without a larval stage.⁴⁶ Its
77 locomotor activity is limited to movements between prey (usually no more than a few centimetres) on which
78 individuals are reported to feed for hours, if not days.⁴⁷ *Nucella lapillus* is only occasionally found below
79 the tide marks and does not voluntarily crawl over sandy or muddy areas. The absence of a larval stage
80 and the limited locomotor range of *N. lapillus* limits its dispersal so that distinct phenotypes exist within
81 different allopatric populations, forming numerous discrete gamodemes.⁴⁸ Its calcareous shell consists of two
82 layers, made of irregular calcite on the outside and crossed lamellar aragonite on the inside, which may
83 be separated by a spherulitic transitional layer.⁴⁹ Site-specific exposure to wave action and predators are
84 the most studied natural causes of shape variability among *N. lapillus* populations.⁵⁰⁻⁵³ On exposed shores,
85 *N. lapillus* usually have short squat shells with a larger aperture size to accommodate a larger foot which
86 improves adherence to substrata. Squatter shells and better substratum adherence reduce the risk of dislodg-
87 ment and are thus interpreted to be a morphological adaptation to increase survival.^{54,55} *Nucella lapillus* on
88 protected shores, where individuals are more regularly exposed to predators, tend to produce stronger and
89 thicker shells^{56,57} and have increased growth rates.⁴¹ Individuals from protected shores also tend to exhibit
90 relatively lighter soft tissue body weight as thicker shells provide comparably less space to accommodate the
91 organism.⁵⁵ Site-specific exposure regimes have also been associated with genetic variability (karyotypes).
92 *Nucella lapillus* show a pronounced chromosomal polymorphism; first reported in populations from the coast
93 of Roscoff, France.⁵⁸ Known chromosome numbers range from $2n = 26$ to $2n = 36$ between populations.^{59,60}
94 It was suggested that karyotypes correlate with local conditions, as the $2n = 26$ karyotype appeared to be
95 more common on exposed shores, whereas the $2n = 36$ karyotype appeared to be more common on protected
96 shores.⁶¹ However, other studies did not confirm this finding, suggesting that shell shape in *N. lapillus* is a
97 direct response to its physical and biological environment, expressed within a single generation and without
98 the need for a change in karyotype.^{62,63} In any case, *N. lapillus* shows pronounced phenotypic adaptations to
99 its habitat allowing this intertidal muricid to become a dominant top-down predator. New and continuous

100 stressors, as brought about by OA and ocean warming, could, however, endanger its position, potentially
101 jeopardising the trophic system on large parts of the North Atlantic rocky shore. While a wealth of stud-
102 ies exists in the literature that examines local effects on *N. lapillus*' shell morphology, comparably little is
103 known about large-scale shape trends, despite its wide distribution. However, this would be of particular
104 interest to understand how this important intertidal predatory gastropod adapts to different environments
105 and has the potential to provide new insights and understanding of this species' capacity to respond to a
106 world in change. This paper aims to close this gap by investigating response patterns of *N. lapillus* across
107 its entire latitudinal dispersal range with a particular focus on identifying significant relationships between
108 environmental gradients and phenotypic responses which may indicate sensitivities of this intertidal muricid
109 to environmental change. To do so, we analysed the shape variance across *N. lapillus* populations, sampled
110 over a 30 degrees latitudinal range, from the northern tip of Norway to the south of Portugal, and used
111 multivariate ecological models to identify significant relationships of shell shape to global change relevant
112 environmental parameters.

113 **Materials and Methods**

114 **Shell collection**

115 Specimens used in this study were sampled from the extensive *Crothers* collection at the Natural History
116 Museum, London, United Kingdom (NHM) (Tab. 1). These samples were collected by John Crothers and
117 colleagues during the 1970s-1980s from numerous sites to study shell shape and colour changes with a special
118 focus on wave exposure levels.⁶⁴⁻⁷⁰ From this collection, we sub-sampled a total of 1575 specimens from 19
119 sites spanning nearly the entire latitudinal range of *N. lapillus* on the European North Atlantic and Arctic
120 coast (Fig. 1). We only included specimens with intact apices that showed no extensive signs of erosion that
121 had likely reached sexual maturity during their lifetime.⁷¹

122 **Environmental descriptors**

123 To study the effect of environmental constraints on shell morphology, we used data from the global ocean-
124 *in-situ* reprocessed carbon observations product (Copernicus Marine Service). This comprehensive global
125 data set contains a compilation of *in-situ* observational gridded data collected from 1950 until 2020 for
126 key parameters such as water temperature, salinity, alkalinity and pH from two up-to-date carbon and
127 biogeochemistry data products, namely the Surface Ocean Carbon Atlas (SOCATv2020) and the Global
128 Ocean Data Analysis Project (GLODAPv2.2020) that underwent rigorous data quality and bias checks.^{72,73}

129 The data has a 1x1 degree spatial resolution at 33 different water depths. For this study, we used only
130 sea surface data to reflect the conditions in the intertidal zone. Seawater conditions used in the further
131 analysis were inferred from the nearest data grid to each sampling site. To have access to all carbonate
132 system parameters, we calculated missing values using pH and alkalinity as input parameters to the function
133 *carb()* in the R package *seacarb* v3.3.0.⁷⁴ The default dissociation constants (K1 and K2) for the respective
134 temperature and salinity ranges were used in the calculation.⁷⁵

135 **Morphometric analysis**

136 We measured standard dimensions, namely shell height, shell width, aperture height and aperture width,
137 using digital Vernier callipers. Every dimension was measured three times per shell. Aperture size was
138 estimated from height and width measurements using the equation for the area of an ellipse. Continuous
139 shell shapes (outlines) were obtained using elliptic Fourier analysis (EFA)^{76,77} using an adaptation of the
140 methodology laid out elsewhere.⁵ For this, shells were individually positioned on an illuminated platform
141 with the aperture facing downward. Images were taken from a fixed distance with a DSLR Camera (Nikon
142 3000, Sigma 105 mm macro lens) mounted on a photo stand in a dark room. This produced images of the
143 shells as black silhouettes with clear outlines, ideal for automatic outline tracing. We decided to analyse
144 shell shape variability with the shell apertures facing downward in a natural position, rather than in the
145 more common but unnatural aperture upwards position, to study shape changes that are more meaningful
146 for *N. lapillus* in nature. Shell silhouette images were imported to R,⁷⁸ and outlines were digitised and
147 subsequently turned into closed shape polygons (defined by x-y coordinates) using the R package *Momocs*.⁷⁹
148 Shape outlines were smoothed using a running average smoothing algorithm to remove digitisation noise
149 before each shell was individually aligned along its longitudinal axis. This was done by defining a secant line
150 that connected the two furthest apart points (i.e., the shell anterior with the posterior) within the polygon
151 shape. The shape was then rotated until the slope of the secant line was zero. Thereafter, shape polygons
152 were centred and scaled with regard to orientation and size. An EFA with 10 harmonics encompassing 99 %
153 of the total harmonic power was computed on the outlines. Principal component analysis (PCA) was used
154 to identify the axes of most variance among individuals (hereafter shape-PCs). For further analyses, we used
155 the first five shape-PCs that encompassed more than 86% of the total shell shape variance among specimens
156 as representative shape descriptors. A graphical representation of the shell shape analysis pipeline can be
157 obtained from the supplementary material. To visualise the transition between extremes of the morphospace,
158 we generated deformation grids⁸⁰ (Fig. 2B) and iso deformation lines⁸¹ (Fig. 4) for each shape-PC. Individual
159 relationships of the first five shell shape descriptors with sampling site latitude were analysed using simple

160 linear regression analyses (Fig. 2).

161 Data analysis and model formation

162 The effect of key environmental parameters on shell shape variability was investigated using generalised addi-
163 tive mixed models (GAMM, *mgcv*)⁸² to accommodate the hierarchical structure and non-linear relationships
164 in our dataset. Initial data exploration was done following the protocol by Zuur et al. (2010).⁸³ No significant
165 outliers were detected among shape-PCs. Boxplots of shape-PCs by sampling sites showed heterogeneous
166 variances between shape-PCs which was an expected consequence of the PCA. Since the aim of this work was
167 to study the effect of global change on shell formation, we considered a range of associated environmental
168 parameters of the physical and chemical domain as model predictors. As stated earlier, Ω_{CaCO_3} states are
169 indicators for spontaneous carbonate precipitation and, as such, have been shown to be good predictors
170 of bio-calcification.⁸⁴ However, apart from the theoretical framework, there is little evidence supporting its
171 mechanistic role in molluscan shell formation.²⁷ There is growing evidence that hydrogencarbonate concen-
172 tration $[HCO_3^-]$ rather than $[CO_3^{2-}]$ is likely the primary carbon species used in bio-calcification.⁸⁵⁻⁸⁸ Thus,
173 we also included the substrate inhibitor ratio (SIR) along with the other parameters as possible predictors
174 to describe variability in the carbonate system that is likely more mechanistically relevant to biological
175 calcification.^{26,27,89} The SIR is a ratio of $[HCO_3^-]$ concentration by proton availability (H^+) in $\text{mol } \mu\text{mol}^{-1}$
176 (eq. 2) and, as such, is a representative of the inorganic carbon substrate availability in relation to precipi-
177 tation conditions.

$$SIR = \frac{[HCO_3^-]}{[H^+]} \quad (2)$$

178 The predictors included in the initial model were: temperature, salinity, total alkalinity (A_T), pH, $[HCO_3^-]$,
179 Ω_{Ar} , Ω_{Ca} , SIR, sampling site ID and shell height. We selected the first three shape-PCs that exhibited
180 a significant correlation with latitude (Fig.2) to be included in the GAMM. Given that all three selected
181 shape-PCs are shape-representatives of the same shell, normalised shape-PC1 to shape-PC3 descriptors
182 were included simultaneously within the same GAMM to allow for a holistic description of the shell shape
183 variability. The number of knots per descriptor was manually defined to constrain unnatural degrees of
184 wiggleness, and cubic regression splines were used. The *dredge()* function in the R package *MuMIn*⁹⁰ was
185 used to analyse all possible combinations of predictors, and the Akaike Information Criterion (AIC) was used
186 as the principal tool in the model optimisation process. To overcome potential complications with collinearity
187 in the model caused by correlated independent variables only models with an acceptable VIF factor < 3 of

188 covariates were considered. The sampling site ID was included as a *random effect* term to account for the
 189 dependency of specimens from the same collection site. The best-supported model was then fitted using
 190 the restricted maximum likelihood approach (REML) and validated by inspection of standardised residual
 191 patterns to verify model assumptions. Variogram inspection suggested no significant spatial autocorrelation.
 192 The final model was of the form:

$$\begin{aligned}
 & \text{shapePC}_{ij} \sim N(\mu_{ij}; \sigma^2) \\
 \mu_{ij} = & f(\text{temperature}_i) * f\text{shape}_j + f(\text{alkalinity}_i) * f\text{shape}_j + f(\text{SIR}_i) * \\
 & f\text{shape}_j + f(\text{shellheight}_i) * f\text{shape}_j + \epsilon_i \\
 & \epsilon_i \sim N(0; \sigma_i^2)
 \end{aligned} \tag{3}$$

193 where shapePC_{ij} represents the j^{th} observation for each shape-PC ($j = 1-3$) at every *sampling site* i ($i =$
 194 $1-19$). $f() * f\text{shape}$ denote the smoothing functions of *temperature*, *alkalinity*, *SIR* and *shell height* expressed
 195 by individual smoother for each level of j and ϵ_i is the normally distributed random intercept. Effect size
 196 estimates of standardised predictors were calculated from the GAMM following Telesca et al. (2018).⁵ The
 197 standardisation of model predictors was done by subtracting the predictor's mean from its standard deviation.
 198 95% confidence intervals were constructed along mean effect sizes to compare the magnitude and significance
 199 of environmental predictors on shell shapes. All exploratory data analyses and modelling were performed in
 200 R⁷⁸ and all data and scripts are publicly available (see data availability statement).

201 Results

202 Mean plots of environmental parameters revealed clear gradients from north to south (Fig. 1). As expected,
 203 mean sea surface temperature increased gradually towards the south. Maximum difference in average tem-
 204 perature between sampling sites was 11.49 °C. Seawater salinity showed an increasing trend towards the
 205 south with pronounced local variability (Fig. 1, sampling sites 7-9). Salinity variations between sampling
 206 sites were up to 3.14 PSU. Seawater pH decreased between 70°N to 50°N, but sampling sites south of 50°N
 207 exhibited higher seawater pH (Fig. 1). The maximum seawater pH range encompassed between our sam-
 208 pling sites was 0.13. Minimum seawater Ω_{Ca} and Ω_{Ar} values at the sampling sites were 3 and 2 respectively.
 209 Seawater Ω_{Ca} states showed no apparent trend over the whole studied latitudinal range but a significant
 210 increase in saturation south of 50°N.

211 Relative contributions of the first five shape-PCs to the total morphospace range are shown in Figure 2B.

212 Overall, shape variance explained by shape-PC1 (53.17 %) was a widening of the shell. Higher shape-PC1
213 values described wider, more globular shells with almost rectangular shoulders and proportionally larger
214 body whorls. Lower values described a narrowing of the shell with proportionally smaller body whorls and
215 flatter shoulders. Shape-PC2 (14.76 %) described a rounding of the body whorl. Higher shape-PC2 values
216 described an overall rounding of the body whorl with a less contoured siphonal canal. Shape-PC3 (8.65
217 %) described an “offsetting” of the body whorl to the spire, which gave the impression of tilting the shell’s
218 longitudinal axis. Shell shape-PC4 (5.94 %) and shape-PC5 (4 %) only explained minor shape variations.
219 Shape-PC4 described a slight widening and shift of the body whorl, especially around the shoulder, and
220 shape-PC5 described contouring of the shell. A plot of among-population variation described by shape-PC1
221 and shape-PC2 showed a clear separation among populations, especially along the shape-PC1 axis (Fig. 3).
222 Mean plots of selected shell descriptors (shape-PC1 to shape-PC5) also showed a clear effect of locality and
223 significant latitudinal trends. Linear regression analyses confirmed significant shell shape changes in relation
224 to sampling site latitude as expressed by shape-PC1, shape-PC2 and shape-PC3. Shape-PC4 and shape-PC5
225 did change significantly with latitude (Fig. 2).

226 The best-supported model (Tab. 2) revealed a significant relationship between the selected shape descriptors
227 and environmental gradients. The model comparison revealed that sea surface temperature, A_T , SIR, shell
228 height, and sampling site ID (as a *random effect* term) best described the observed changes in shape-PCs.
229 The model identified highly significant non-linear relationships of shape-PC1 with sea surface temperature,
230 A_T , SIR and shell height (Fig. 4A). Shape-PC2 showed a non-significant relationship with sea surface
231 temperature but highly significant relationships with A_T and SIR. Shell height had only a minor effect on
232 shape-PC2 (Fig. 4B). Shell shape variance described by shape-PC3 was also not associated with sea surface
233 temperature but showed significant correlations with A_T , SIR and shell height (Fig. 4C). Mean effect size
234 estimates (Fig. 5) revealed differences in the relative contribution of environmental predictors on observed
235 changes in shape. The SIR and shell height showed a significant effect on shell shape-PC1 to shape-PC3,
236 and in addition, A_T exhibited a significant effect size for shape-PC2. Overall, effect size estimates primarily
237 linked changes in the carbonate system as represented by A_T and especially the SIR to changes in shell shape.
238 Most notably, we identified the formation of wider, more globular shells with a more pronounced shoulder
239 with increasing SIR values. Effect size estimates for sea surface temperature were non-significant for any of
240 the three shape descriptors.

241 Discussion

242 Using a combined EFA and GAMM approach, we identified significant shape changes in the intertidal *N.*
243 *lapillus* that followed latitudinally (Fig. 2) and environmental trends (Fig. 4,5). We identified a significant
244 narrowing of shells (i.e., a reduction in the shell aspect ratio) with relatively smaller body whorls from north
245 to south. While we did not identify microclimate effects of individual sites on shell formation, which likely
246 contributed to the observed considerable shape variation between individuals from the same population
247 (Fig. 2), our large scale trends are so clear that the variability of mean environmental conditions among
248 sampling sites must have been significant enough to influence the shell formation in the studied specimens.
249 Although the intertidal zone is known to exhibit pronounced temporal and spatial variability in the carbonate
250 system,⁹¹ our results suggest that a shift in the mean has a significant influence on shell formation. Effect size
251 estimates of environmental predictors on shape-PCs revealed that differences in the carbonate system had
252 the strongest influence of all environmental predictors on shell shape. In contrast, sea surface temperature
253 showed a non-significant effect size for any of the three shape-PCs (Fig. 5). Despite overall high Ω_{Ca} and Ω_{Ar}
254 throughout the sampling sites, shell formation of *N. lapillus* appears to be remarkably sensitive to variations
255 in the carbonate system. Our models indicate a significant link between shell formation of *N. lapillus* to
256 variations in the “reactant” $[HCO_3^-]$ and “inhibitor” $[H^+]$ ratio (SIR)^{89,92,93}, which is expected to decrease in
257 the coming years and centuries under increasing OA conditions. This suggests an overall shift in *N. lapillus*
258 shell shape can be expected as a response or consequence to changing water chemistry constraints.

259 There is only a handful of studies explicitly investigating shell shape responses of marine gastropods to
260 changes in the carbonate system, and these have produced partly conflicting results. A study of the shell
261 aspect ratio in the gastropod *Phorcus sauciatius* collected from a CO_2 vent and a control site reported
262 a similar shape response to those here, as specimens from the vent site tend to form narrower and more
263 elongated shells.¹⁹ However, seemingly conflicting results were reported from laboratory studies where the
264 combined effect of increasing seawater temperature and decreasing pH resulted in the formation of more
265 globular shells in the intertidal gastropod *Littorina littorea* and in juvenile *N. lapillus*.^{94,95} This discrepancy
266 among studies is not easily resolved but highlights the complexity of comparing species responses from
267 laboratory and field studies. One of the biggest issues in comparing gastropod shape studies is the lack
268 of a common vocabulary and methodology to describe shape responses. One prominent example here is
269 the interchangeability of the words “globular”, “wide”, “spherical”, “squat”, “round” to describe seemingly
270 similar shape changes for which a visual representation of morphospace extremes (Fig. 2B and Fig. 5) would
271 provide a better basis of comparison.

272 The discrepancy between study results also raises the interesting question of whether a universal shape
273 response to changing water chemistry can be expected or if different species will respond in different ways
274 to OA. A crucial point when shell shape responses to a variable carbonate system are to be compared is
275 the careful separation between kinetically, thermodynamically, and stress-induced shape alterations, or in
276 other words, if the phenotypic response is adaptive or non-adaptive. At the simplest level, changes in the
277 seawater carbonate system as brought about by OA result in a reduction of the bio-calcification substrate
278 accompanied by increases in $[H^+]$ abundance that may constrain crystal formation at the site of calcification
279 through lowering Ω_{CaCO_3} .^{18,26} This means that less material or substrate is available to the individual
280 for shell formation and that calcification likely becomes metabolically more expensive as the individual is
281 required to spend more energy on $[H^+]$ extrusion.^{18,96} While the latitudinal shape trends observed in our
282 study are purely kinetically induced (in accordance with the kinetic–energetic hypothesis)²⁵ and are therefore
283 a direct indicator for variations in substrate and inhibitor abundance, we hypothesise that shape variation
284 in OA laboratory studies is likely a mix of kinetic-, dissolution-, and stress-induced phenotypic responses
285 precluding any direct comparisons.

286 The literature provides a wealth of information about local effects on *N. lapillus* shell shape. Shell aspect
287 ratio variations in relation to local wave exposure regimes were first reported by Cooke (1895).⁹⁷ The author
288 found that *N. lapillus* on exposed shores exhibited smaller, squatter shells with a larger aspect ratio, whereas
289 individuals from protected shores formed narrower, more elongated shells. This trend was later explained
290 to be a response that improved fitness as smaller squatter shells and a proportionally larger foot of exposed
291 individuals (obvious from relatively larger aperture sizes) conferred an advantage over more elongated shell
292 forms with smaller foot sizes in high wave energy environments.⁹⁸ However, the exposed morph showed a
293 marked disadvantage on sheltered shores as animals of that shell form could barely retract into the shell,
294 making them more vulnerable to predators and desiccation during low tide.⁹⁹ Crothers (1973) found the shell
295 height to aperture height ratio to be a convenient proxy for wave exposure trends for *N. lapillus* populations
296 on Pembrokeshire, UK shores and thereby quantified the relationship between wave exposure and relative
297 aperture size.¹⁰⁰ However, unlike the reported wave exposure induced shape changes, mean shape-PCs in
298 this study showed no relationships with aperture size (Fig. 6). Likewise, we also did not observe a change
299 in apertural teeth expression across studied populations which would indicate variations in wave exposure⁶⁴
300 or predatory pressure⁵⁷ constraints on shell deposition in the studied *N. lapillus* populations. This suggests
301 to us that shape variations, as explained by shape-PC1 to shape-PC3 (over these large spatial scales), were
302 largely decoupled from local wave exposure and predation gradients.

303 While shape variations are an excellent proxy to identify new or changing environmental stressors in a

304 population or species,¹⁰¹ predictions of the long term consequences of plastic adaptations are not trivial - or
305 to use the words of R. J. Berry and J. H. Crothers: “*Natural populations of animals rarely behave like*
306 *suspensions of inanimate matter in a frictionless fluid, responding to and predictable by simple mathematical*
307 *theory*”.⁴⁸ However, newly introduced stressors and associated phenotypic adaptations always represent a trade-
308 off between different optima and can thus challenge an organism’s position in an ecosystem.¹⁰² Our findings
309 suggest that a trend toward narrower, more elongated shells can be expected under increasing OA conditions
310 with, perhaps, significant implications for the predator-prey relationship on North Atlantic rocky shores.
311 Although shape-PCs were largely decoupled from local wave exposure gradients, a continuing trend towards
312 the formation of narrower and more elongated shells could have conceivable consequences for populations on
313 (extremely) exposed coasts. In particular, since global climate change is associated with increasingly severe
314 storm events,¹⁰³ the larger surface of elongated shells could lead to more frequent dislodgement and, as a
315 consequence, could make *N. lapillus* populations more susceptible to predatory attacks. The herein observed
316 shell shape response to OA could lead to a disintegration of the delicate balance between shape responses
317 to wave exposure or predatory pressure extremes with the potential consequence of a realignment of rocky-
318 shore community structures. However, our results and predictions of morphological responses to end century
319 OA conditions should be viewed with caution for three reasons: First, the site-specific intra-population
320 variability is many times larger than the average shift in shape observed in this study (Fig. 2), suggesting
321 that there is a fair amount of tolerance involved in the shape response to environmental constraints. Second,
322 a sensitivity analysis of shell morphology to different stressors is missing, which would be required to make
323 robust predictions. Third, temporal and spatial constraints of environmental data used in this study limited
324 fine-scale observations. While our models suggest a remarkable sensitivity of shell shape to variations in the
325 carbonate system on a large geographic scale, it is not clear if shell morphology will be more sensitive to
326 water chemistry or site-specific physical constraints under increasing OA conditions.

327 Irrespective of the direct consequences, our results show that changes in the carbonate system are likely
328 to directly affect *N. lapillus* shell morphology. Although calcification conditions were, in classical terms,
329 favourable at every sampling site, shell formation and resulting morphology were sensitive to changes in the
330 SIR. Our findings uncovered a, so far unrecognised, large scale pattern in shell morphology of the intertidal
331 *N. lapillus*, which highlights the coupling of phenotypic adaptations to variations in the carbonate system.
332 However, although our findings suggest an adaptive trend in shell morphology under increasing OA conditions,
333 further research is required to understand the phenotypic sensitivity to local and global constraints, which
334 could present an exciting new research opportunity to understand shell formation constraints in a changing
335 world.

336 Data availability

337 All data and code used in this study are made publicly available on the following Github repository:
338 dm807cam/nucella2021world.

339 Tables

Table 1: Sampling details of the *Nucella lapillus* shells used in this study. For each sampling site the number of specimens, their respective mean shell height and standard deviation are reported. Only specimens with clearly identifiable sampling site were used. Sampling sites are sorted by latitude from north to south.

ID	site	coordinates	individuals	mean shell height (mm)	var. shell height (1σ)
1	Bjarkøy	68.99 °N, 16.54 °E	48	29.56	2.87
2	Litløya	68.59 °N, 14.32 °E	53	28.52	3.19
3	Fljótavík	66.45 °N, 22.91 °W	97	30.34	2.29
4	Lurøy	66.37 °N, 12.6 °E	99	32.36	2.19
5	Tjørnuvík	62.3 °N, 7.14 °W	50	32.35	3.25
6	Suðuroy	61.52 °N, 6.78 °W	48	37.75	3.98
7	Hoplandsjøen (Harbour)	60.75 °N, 4.91 °E	94	31.89	2.64
8	Hoplandsjøen (outer)	60.75 °N, 4.91 °E	99	29.14	2.14
9	Ramsøy	60.44 °N, 5.05 °E	49	33.31	2.82
10	Mavis Grind (East)	60.39 °N, 1.38 °W	51	31.02	1.93
11	Voe	60.27 °N, 1.16 °W	101	28.81	2.92
12	St Abbs	55.89 °N, 2.12 °W	104	31.37	2.68
13	Berwick upon Tweed	55.77 °N, 1.99 °W	100	28.88	2.35
14	Mumbles	51.56 °N, 3.98 °W	96	32.75	2.02
15	Shoreham (Harbour)	50.82 °N, 0.25 °W	101	33.98	2.76
16	Ile de Batz	48.75 °N, 4.01 °W	88	31.80	2.41
17	Quiberon (Port Haliguen)	47.49 °N, 3.1 °W	100	29.21	2.09
18	Redondela	42.29 °N, 8.63 °W	101	33.69	1.88
19	São Martinho do Porto	39.52 °N, 9.14 °W	99	26.43	1.31

Table 2: GAMM summary statistics of the best supported model. Estimated degrees of freedom, F statistics and significance values for each predictor variable are reported.

Shape-PCs	Temperature			Alkalinity			SIR			Shell height			Site		
	edf	F	<i>p</i>	edf	F	<i>p</i>	edf	F	<i>p</i>	edf	F	<i>p</i>	edf	F	<i>p</i>
PC1	1.978	23.012	< 0.001	1.887	4.214	0.014	1.959	23.712	< 0.001	1.897	199.049	< 0.001	13.521	15.731	< 0.001
PC2	1.813	2.877	0.11	1.000	14.893	< 0.001	1.813	14.488	< 0.001	1.799	3.399	0.023	13.521	15.731	< 0.001
PC3	1.592	3.070	0.138	1.970	17.961	< 0.001	1.001	4.116	0.042	1.001	72.436	< 0.001	13.521	15.731	< 0.001

Figures

Figure 1: Sampling map of *Nucella lapillus* specimens and environmental gradients of sea surface temperature, seawater salinity, pH and Ω_{Ca} . The sampling sites ranged from 40°N to almost 70°N spanning three distinct climate zones. Names of corresponding sampling site IDs can be obtained from Table 1. The colour gradient in the sampling map corresponds to that in the temperature plot, and all gradient colours are in accordance with Thyng et al. (2016).¹⁰⁴

Figure 2: (A) Latitudinal trends of shell shape descriptors (shape-PC1 to shape-PC5) of the intertidal gastropod *Nucella lapillus*. Points represent the mean at every sampling site, and error bars denote the standard deviation. Linear regression significances are reported for each shape-PCs (Significance levels: n.s. $p > 0.05$, * $p < 0.05$, ** $p < 0.001$, ***, $p < 0.0001$). (B) Deformation grids of shape-PC1 to shape-PC5 visualising the transition between extremes of the morphospace represented by each shape-PCs (blue: mean - 3σ , red: mean + 3σ). Percentage contributions to total shape variance between individuals are reported for each shape-PC.

Figure 3: Scatter plot of the first two shape-PCs from PCA analysis performed on elliptic Fourier coefficients revealing the among-population variation of outline and shape features between *Nucella lapillus* specimens. Confidence intervals are shown for each origin group (ellipses with dashed linetype), and corresponding morphospace extremes are represented as grey shapes.

Figure 4: GAMM shape trend predictions of the best-supported model as expressed by shape-PC1 to shape-PC3 with selected descriptors of sea surface temperature, A_T and substrate inhibitor ratio (SIR) and normalized shell height. Significance is reported for each predictor (Significance levels: n.s. $p > 0.05$, * $p < 0.05$, ** $p < 0.001$, ***, $p < 0.0001$). Colour gradients (red to blue) of significant predictor terms correspond to those in Figure 5.

362 Figure 5: Iso deformation lines of shape-PC1 to shape-PC3 and the best-supported model's mean effect size
363 plots, including sea surface temperature, A_T , substrate inhibitor ratio (SIR) and shell height. Error bars
364 represent the 95% CI, and the significance of either predictor is determined if the CI does not cross the
365 zero line ($p < 0.01$). Asterisks mark significant predictors. Colour gradients (red to blue) correspond to the
366 morphospace extremes visualised to the left of each effect size plot.

367 Figure 6: Correlation plot of mean aperture size vs mean shape-PCs grouped by sampling site. Error bars
368 denote the standard deviation. The orange dashed line represents the 1:1 correlation line.

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