

1 **Computational Fluid Dynamics Suggests Ecological Diversification among Stem-**
2 **Gnathostomes**

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25 **SUMMARY**

26 **The evolutionary assembly of the vertebrate bodyplan has been characterised as a long-**
27 **term ecological trend towards increasingly active and predatory lifestyles, culminating in**
28 **jawed vertebrates which dominate modern vertebrate biodiversity [1–8]. This contrast is**
29 **no more stark than between the earliest jawed vertebrates and their immediate relatives,**
30 **the extinct jawless, dermal armour-encased osteostracans, which have conventionally been**
31 **interpreted as benthic mud-grubbers with poor swimming capabilities, and low**
32 **manoeuvrability [9–12]. Using computational fluid dynamics, we show that osteostracan**
33 **headshield morphology is compatible with a diversity of hydrodynamic efficiencies**
34 **including passive control of water flow around the body; these could have increased**
35 **versatility for adopting diverse locomotor strategies. Hydrodynamic performance varies**
36 **with morphology, proximity to the substrate and angle of attack (inclination). Morphotypes**
37 **with dorsoventrally oblate headshields are hydrodynamically more efficient when**
38 **swimming close to the substrate, whereas those with dorsoventrally more prolate**
39 **headshields exhibit maximum hydrodynamic efficiency when swimming free from**
40 **substrate effects. These results suggest different hydrofoil functions among osteostracan**
41 **headshield morphologies, compatible with ecological diversification and undermining the**
42 **traditional view that jawless stem-gnathostomes were ecologically constrained [9–12] with**
43 **the origin of jaws as the key innovation that precipitated the ecological diversification of**
44 **the group [13,14].**

45

46 **RESULTS**

47 The origin of vertebrates can be characterised by increased cephalisation and a number of
48 developmental and anatomical innovations rooted in whole genome duplication, increased

49 gene regulation, and the diversification of neural crest cell fates [15–17]. The ecological
50 context to this formative evolutionary episode is envisioned as successive evolutionary grades
51 of invertebrate chordates, jawless vertebrates and jawed vertebrates, exhibiting an overall
52 trend towards increasingly active food acquisition that culminated in the active predatory
53 ecology of extant gnathostomes [3,4]. In this scenario, the extinct jawless ‘ostracoderms’ are
54 interpreted as cumbersome deposit feeders lacking key apomorphies of jawed vertebrates
55 including multiple pairs of appendages and an epicercal tail, as well as jaws. This popular
56 scenario belies the challenge of constraining the biology of ostracoderms which lack living
57 analogues, traditionally compromising attempts to derive functional interpretations of their
58 morphology [18]. However, the development of non-destructive tomographic methods for
59 characterizing morphology, combined with computational engineering approaches that can
60 be used to analyse quantitatively the functional performance of biological structures [19,20],
61 render such macroecological and macroevolutionary hypotheses testable.

62

63 To this end, we analysed the functional morphological diversity of the Silurian–Devonian
64 Osteostraci, the jawless sister group to all jawed vertebrates, which cover all the
65 morphological grades exhibited by ostracoderms, including forms which entirely lack paired
66 appendages and others that possess just a single (pectoral) pair (Figure 1a). The generic semi-
67 circular, dorsoventrally flattened (oblate) osteostracan headshield has conventionally been
68 interpreted as an adaptation to a sedentary benthic ecology [10,11,21–24]. However,
69 osteostracan cranial morphology exhibits greater morphological disparity, including:
70 morphotypes that are laterally compressed (prolate) and lack pectoral fins, interpreted as
71 adaptations for burrowing, as well as forms with lateral and rostral expansions of the
72 headshield, interpreted as adaptations for stabilization, enhancing lift or reducing drag

73 [12,23,25], deterring predators [26], housing sense organs [27], substrate anchoring [28], or
74 specialised feeding strategies [29]. Using geometric morphometrics, we characterized
75 quantitatively the morphological diversity of osteostracan headshields and derived an
76 empirical morphospace that we interrogated using computational fluid dynamics (CFD) to
77 determine how variation in morphological disparity correlates to aspects of hydrodynamic
78 performance. CFD allowed us to simulate the interaction between flow and digital models of
79 osteostracan morphology in three dimensions, exploring not only the impact of differences in
80 morphology, but also the attitude of the organism with respect to flow (angle of attack) and
81 its position relative to the substrate. We explored the fluid flow and forces generated over
82 static models, interpreting the results exclusively in terms of morphological variation and
83 assuming comparable modes of locomotion and post-cranial morphology for all species. The
84 post-cranial anatomy of osteostracans is relatively conservative [18] and, hence, our
85 morphospace analysis focussed on the headshields. In this way, we were able to test
86 competing hypotheses of osteostracan ecology based on hydrodynamic performance criteria
87 (such as the lift-to-drag ratio).

88

89 We characterised headshield morphology for 30 species belonging to 29 different genera and
90 representing all major groups and the systematic breadth of osteostracans, using 123
91 landmarks of type I–III (Figure 1b), which were subjected to Procrustes and pairwise distance
92 analysis prior to ordination. The ensuing phylomorphospace conveys the relationship
93 between phylogeny and morphological variation (Figure 1c), revealing widespread
94 convergence evidenced by many pairs of taxa that are morphologically more similar than
95 either are to their last shared ancestor. We applied CFD to eight taxa sampled from the limits
96 of morphospace occupation, as well as the most common morphologies (Figure 1c).

97

98 We simulated both pelagic and benthic conditions with an inlet velocity of 0.3 m s^{-1} . In the
99 pelagic scenario, eight different angles of attack were simulated at 10° intervals between 0°
100 and 70° . In the benthic scenario, the models were positioned at three different distances
101 above the substrate (0.1, 0.5 and 1 body lengths) (Figure 1d). This combination of parameters
102 covers a wide range of hypothetical modes of life, allowing us to interpret the hydrodynamic
103 performance of osteostracan headshield under different ecological scenarios. Results of the
104 simulations were interpreted both qualitatively, by visualizing the pressure distribution at the
105 surface of the body, and quantitatively, by calculating drag and lift coefficients, and lift-to-
106 drag ratios.

107

108 Sensitivity analyses demonstrate that the CFD results are independent of domain and mesh
109 size (see Data S1 and STAR Methods section, respectively). The distributions of pressure over
110 the body vary considerably between the pelagic and benthic simulations (Figure 2). In the
111 pelagic simulations, the highest pressures are restricted to the front of the snout, whereas in
112 the benthic simulations they occur along part of the ventral surface of the headshield. These
113 differences are especially extreme in dorsoventrally compressed morphotypes, such as
114 *Stensiopelta* (Figure 2F) and *Boreaspis* (Figure 2H).

115

116 The drag coefficient (C_D) increases with the angle of attack and proximity to the substrate
117 (Figure 3 and Table S1), showing a positive correlation with the degree of development of
118 headshield cornual processes, in both benthic and pelagic scenarios at low angles of attack
119 (i.e., from 0° to 20°). Under pelagic conditions, the lift coefficient (C_L) increases approximately
120 linearly with angle of attack from 0° to 30° (Figure 3 and Table S1), exhibiting a significant

121 correlation with headshield morphology at low angles of attack (i.e., from 0° to 20°) where
122 the highest values are attained by the morphotypes that are more triangular in outline. C_L
123 achieves its acme at 40°-50° before reaching the critical or stall angle of attack, at which point
124 C_L experiences an abrupt decrease. In the benthic scenario, C_L increases greatly for all
125 morphotypes when they are located close to the substrate, but this effect is especially
126 pronounced in taxa with oblate headshields; otherwise, there is no significant correlation with
127 headshield shape. Absolute lift force generally overcomes apparent weight for all taxa at
128 realistic angles of attack (between 10° and 30°) and cruising swimming speeds (0.30 m s^{-1}) in
129 the pelagic scenario (Table S1). Moreover, the extra lift force generated when the models are
130 located close to the substrate is enough to counteract the apparent body weight for most of
131 the species at an angle of attack of 0°. The ratio between the lift and drag coefficients (L/D)
132 is widely considered as a good proxy for hydrodynamic efficiency, and this varies substantially
133 among the different morphotypes and ecological scenarios in our study (Figure 3 and Table
134 S1). Under the pelagic scenario, the maximum L/D is attained for all morphotypes at angles
135 of attack between 20° and 30° (except for *Hoelaspis* where it is attained at 40°). Under
136 benthic conditions, peak L/D is achieved for all morphotypes when they are located at 0.1
137 body lengths above the floor. Most species with dorso-ventrally oblate headshields show the
138 highest L/D under benthic scenarios, whereas more dorso-ventrally prolate morphotypes
139 achieve peak L/D under pelagic conditions. Morphologically intermediate species do not show
140 major differences between the two scenarios and *Hoelaspis* presents the lowest L/D values in
141 all cases.

142

143 **DISCUSSION**

144 Our analyses indicate that osteostracans with oblate headshields were hydrodynamically
145 more efficient (i.e., they maximized lift and minimized drag) when swimming close to the
146 substrate, whereas prolate morphotypes exhibited maximum hydrodynamic efficiency when
147 swimming in the water column above substrate effects. We also show that headshield
148 morphology in several osteostracan species is compatible with passive control of
149 hydrodynamic performance through ground effect, generating extra lift when swimming
150 close to the substrate that overcame the apparent weight of the fish. This phenomenon is
151 widely used by modern demersal taxa (e.g., flatfishes, skates and rays) to augment lift and
152 counteract negative buoyancy when actively swimming near the bottom [30], occurring as a
153 consequence of the distortion of the flow and the resulting increased pressure below the
154 organism. Patterns of variation in surface pressure (Figure 2) and lift coefficients (Figure 3) for
155 both pelagic and benthic scenarios are also compatible with these osteostracans benefitting
156 from ground effect during active swimming. Some living armoured benthic fishes use similar
157 strategies to counteract negative buoyancy, exploiting ground effect when moving close to
158 the substrate and generating lift by increasing the angle of attack when swimming in more
159 pelagic conditions [31]. This could also be the case for some osteostracans, especially species
160 with oblate headshield morphologies that produce the most lift through ground effect. Oblate
161 cambered bodies (i.e., those with flat ventral sides) might also reflect other lifestyle functions,
162 such as benthic station-holding. On the other hand, hydrodynamic performances calculated
163 for prolate species may reflect strictly pelagic live styles, even when swimming at
164 comparatively low speeds and high angles of attack [32]. In this sense, there are well reported
165 cases of pelagic living fishes, with body sizes and swimming speeds comparable to those of
166 osteostracans, that are able to swim at high angles of attack to counteract negative buoyancy
167 in the water column.

168

169 Our results suggest that the broad disparity and widespread convergence in headshield
170 morphology exhibited by clades of stem-gnathostomes [18] can be explained as a
171 consequence of their hydrodynamic and ecological disparity [12]. This interpretation relies on
172 the assumption of a similar range of body densities for the analysed taxa. Analyses of extant
173 species have shown that cephalofoil function can be complex, and its hydrodynamic role is
174 controversial. In this sense, an alternative scenario of lift generation, compensating for higher
175 density in taxa with larger bony carapaces, should be also considered. However, this view is
176 challenged by the observation that more robust osteostracan headshield morphologies (e.g.,
177 *Stensiopelta*) do not produce greater lift than taxa with more gracile headshields (e.g.,
178 *Hemicyclaspis* or *Cephalaspis*) [33]. Thus, we provide experimental evidence compatible with
179 both ecological diversification and exploration of complex morpho-functional hydrodynamic
180 adaptations among jawless stem-gnathostomes. Indeed, our novel results, coupled with
181 previous research in bioengineering [34] and functional morphology [35], further suggest that
182 mechanisms for passively controlling flow around the body may be prevalent among these
183 groups, where they would have conferred greater manoeuvrability and versatility than
184 previously thought [9–12]. This calls into question the prevailing view that stem-
185 gnathostomes were ecologically constrained prior to the emergence of jawed vertebrates and
186 the scenario of a general trend towards increasingly active food acquisition [3,4]. In this light,
187 the ecology of early vertebrates appears to have been more diverse and complex [36,37].
188 Thus, we have presented evidence of adaptations to a range of different lifestyles and
189 ecologies evolved among jawless stem-gnathostome groups before the origin of jaws,
190 underpinning the later exploration of novel trophic strategies and enhanced locomotory
191 capabilities that emerged with the evolution of jaws, pelvic fins and trunk musculature

192 [14,38,39].

193

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199

200 **AUTHOR CONTRIBUTIONS**

201 P.C.J.D, H.G.F and H.B. devised the project. H.G.F., I.A.R. and C.M.P. designed and performed
202 the simulations. V.S.L. performed the 3D modelling. H.G.F and P.C.J.D wrote the manuscript
203 with the support of the other authors.

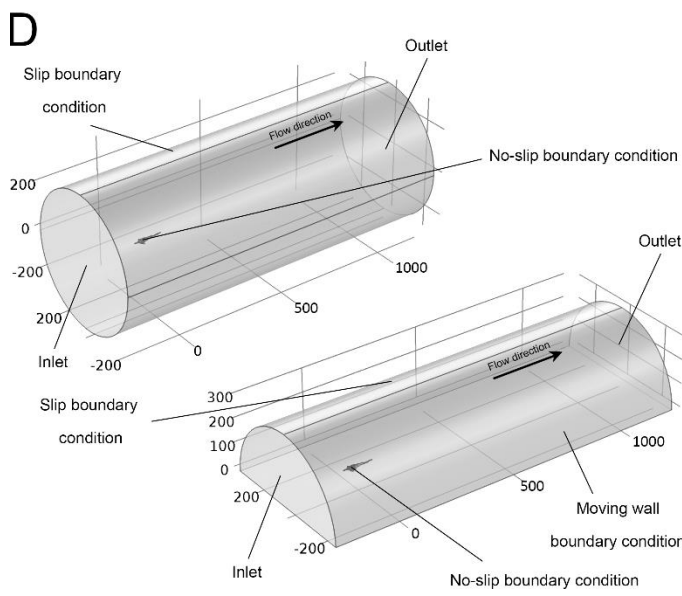
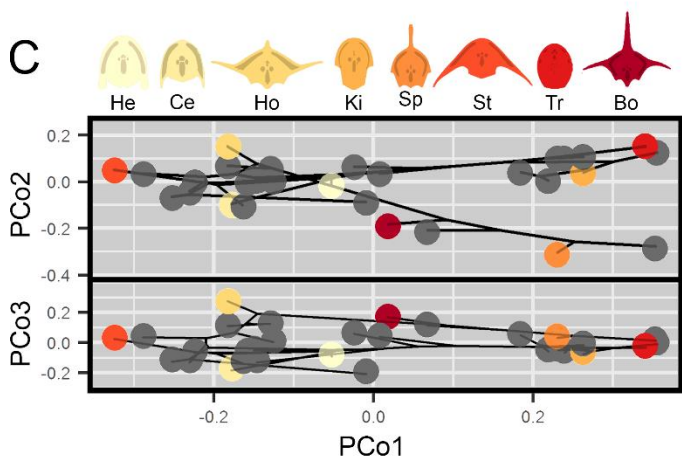
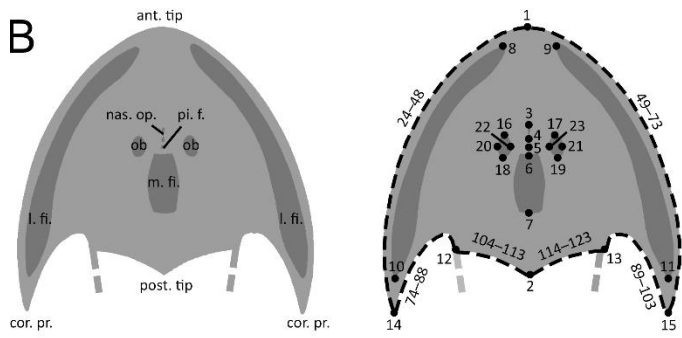
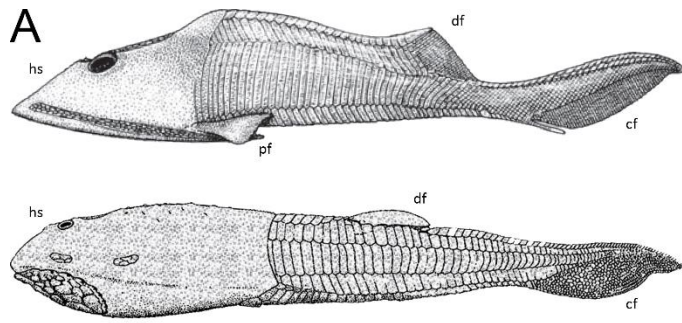
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205 **DECLARATION OF INTERESTS**

206 The authors declare no competing interests.

207

208 **FIGURE LEGENDS**



210 **Figure 1. Morphology of osteostracans and experimental setup.** (A) General morphology of
211 two well-known osteostracans, *Hemicyclaspis* (top) and *Tremataspis* (bottom), in lateral view,
212 indicating the position of the pectoral fins (pf), dorsal fin (df), caudal fin (cf) and headshield
213 (hs). Modified from Janvier [18]. (B) Descriptive diagrams showing anatomical characters of
214 the osteostracan headshield (left) and the landmark configuration used in the geometric
215 morphometric analysis (right). Landmark 1, anterior tip of the headshield or the rostral
216 process (ant. tip.). Landmark 2, posterior tip of the headshield (post. tip.). Landmarks 3 and
217 4, most anterior and most posterior medial points of the nasohypophysial opening (nas. op.)
218 respectively. Landmark 5, pineal foramen (pi. f.). Landmarks 6 and 7, most anterior and most
219 posterior medial points of the median field (m. fi.) respectively. Landmarks 8 and 9, most
220 anterior points of the left and right lateral fields (l. fi.) respectively. Landmarks 10 and 11,
221 most posterior points of the left and right lateral fields (l. fi.) respectively. Landmarks 12 and
222 13, left and right points of connection between the headshield and the body respectively.
223 Landmarks 14 and 15, left and right most distal points of the corneal processes (cor. pr.)
224 respectively. Landmarks 16–23, most anterior, posterior, lateral and medial points of the eye
225 orbits (ob.). Landmarks 24–73, type III landmarks situated between Landmarks 1 and 14 and
226 between Landmarks 1 and 15. Landmarks 74–103, type III landmarks situated between
227 Landmarks 14 and 12 and between Landmarks 15 and 13. Landmarks 104–123, type III
228 landmarks situated between Landmarks 12 and 2 and between Landmarks 13 and 2. Modified
229 from Ferrón et al. [41]. (C) Phylomorphospace summarizing the morphological diversity of
230 osteostracan headshields. The proportion of variance explained by PCo1–3 are 62.46%,
231 17.49% and 12.18% respectively. Taxa used in CFD analyses are highlighted in colour. Bo,
232 *Boreaspis*; Ce, *Cephalaspis*; He, *Hemicyclaspis*; Ho, *Hoelaspis*; Ki, *Kiaeraspis*; Sp, *Spatulaspis*;
233 St, *Stensiopelta*; Tr, *Tremataspis*. (D) Schematic illustration of the computational domain (i.e.,

234 all the objects around/through which the fluid will flow) used in CFD simulations for pelagic
235 (upper) and benthic (lower) scenarios. All measurements in mm.

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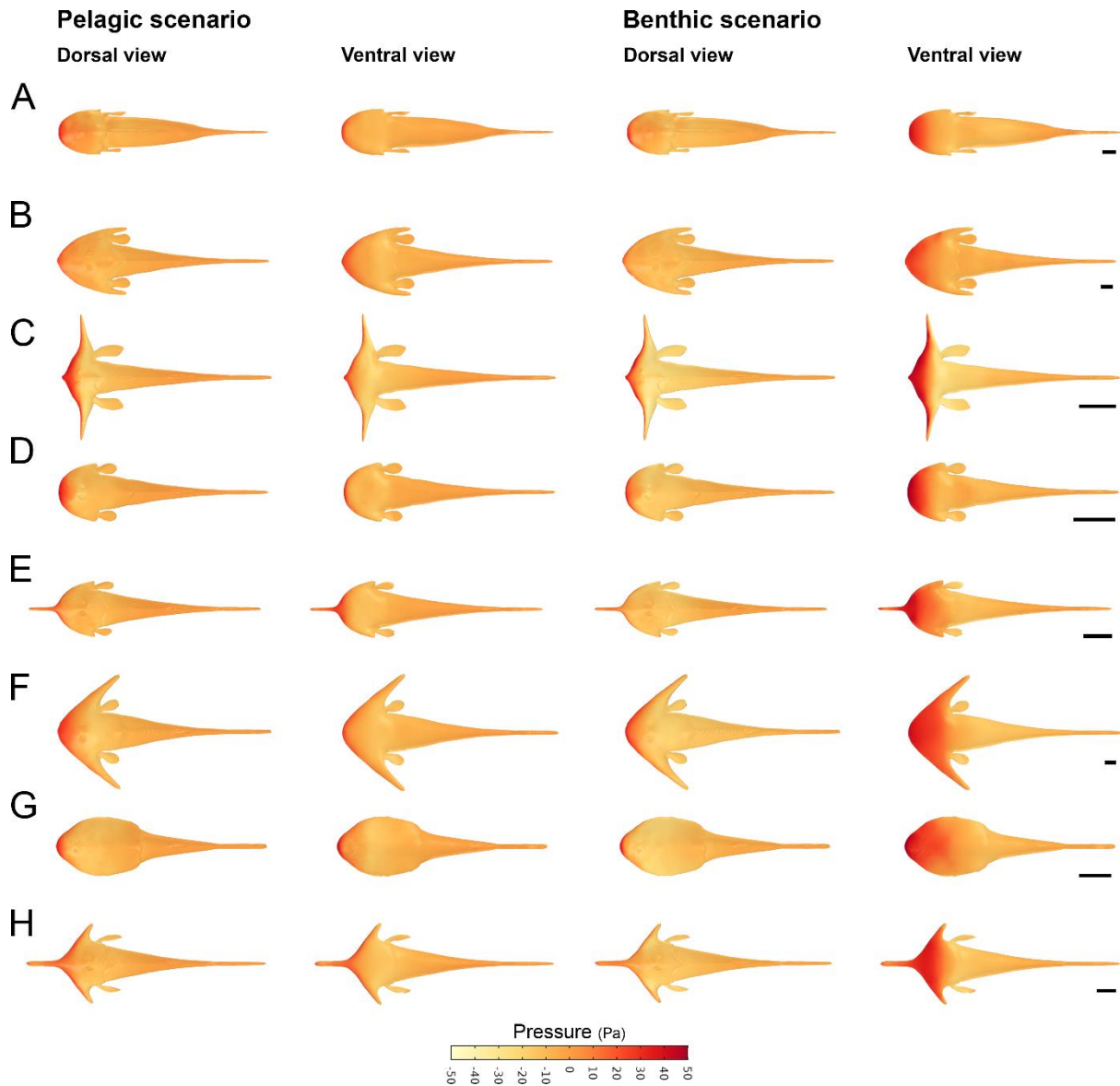
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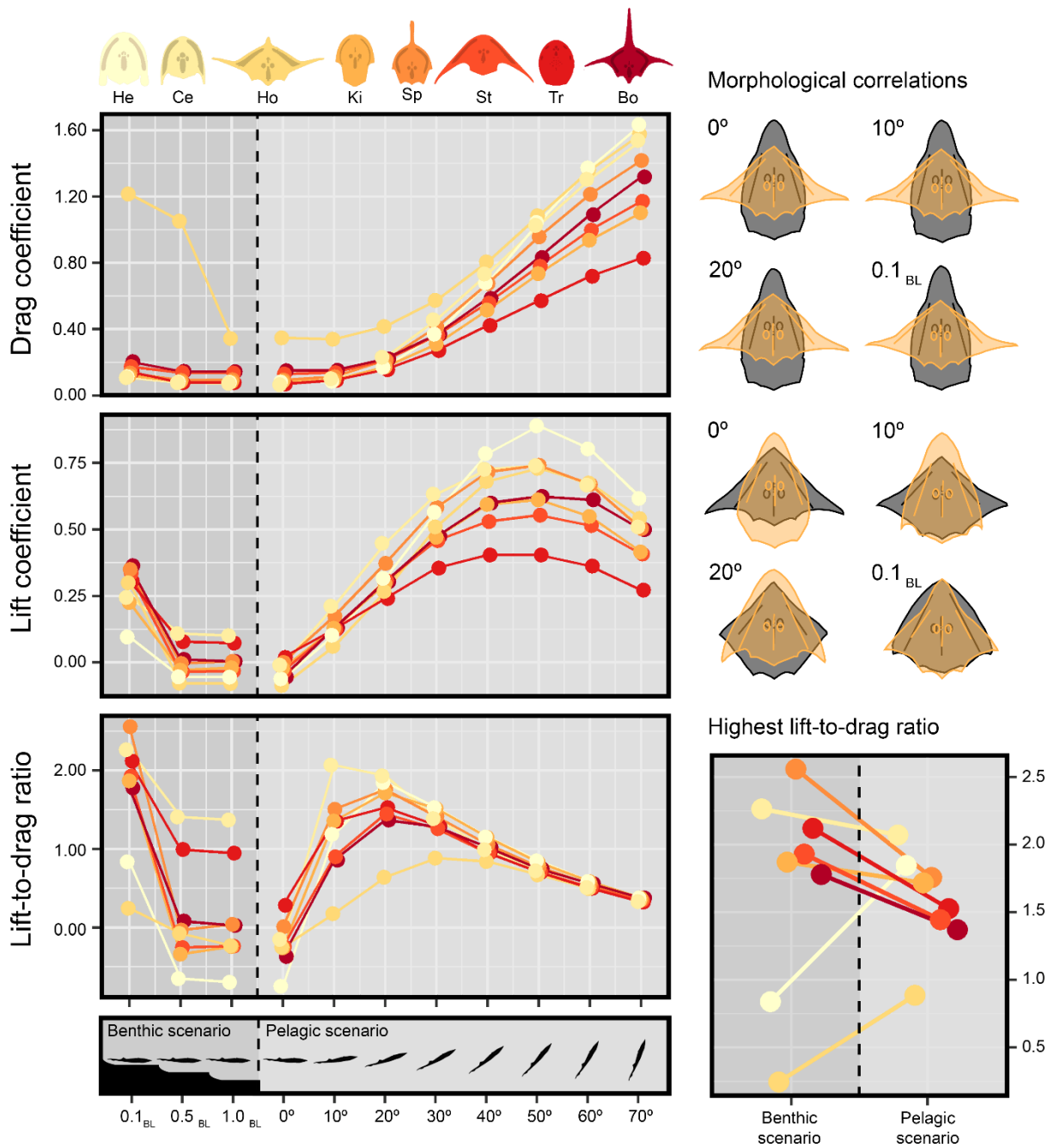
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Figure 2. Results of CFD simulations showing surface pressure distributions for osteostracan models under benthic (distance above the substrate of 0.1 body lengths) and pelagic scenarios (angle of attack of 0°) with an inlet velocity of 0.3 m s⁻¹. (A) *Hemicyclaspis*. (B) *Cephalaspis*. (C) *Hoelaspis*. (D) *Kiaeraspis*. (E) *Spatulaspis*. (F) *Stensiopelta*. (G) *Tremataspis*. (H) *Boreaspis*. Note that models are lit from the top left to reveal their three-dimensional shape, but all of them display symmetrical pressure distribution patterns. Scale bar 2 cm.



250

251 **Figure 3. Results of CFD simulations showing drag and lift coefficients and the lift-to-drag**

252 **ratio, together with associated morphological correlations, under different experimental**

253 **conditions (benthic scenario at 0.1, 0.5 and 1.0 body lengths (BL) above the substrate; and**

254 **pelagic scenario at angles of attack of 0°–70°) with an inlet velocity of 0.3 m s⁻¹. Data**

255 **represented by points correspond to measured values. In the top right panel, grey and orange**

256 **landmark wireframe configurations represent headshield morphologies with higher and**

257 lower force coefficients, respectively. Correlation results: C_D (0°): % predicted = 42.28, p-value
258 = 0.0005; C_D (10°): % predicted = 42.16, p-value = 0.0001; C_D (20°): % predicted = 41.06, p-
259 value = 0.0003; C_D (0.1_{BL}): % predicted = 34.28, p-value = 0.0077; C_L (0°): % predicted = 42.15,
260 p-value = 0.0012; C_L (10°): % predicted = 21.07, p-value = 0.0544; C_L (20°): % predicted =
261 22.48, p-value = 0.0518; C_L (0.1_{BL}): % predicted = 3.01, p-value = 0.6921. Bo, *Boreaspis*; Ce,
262 *Cephalaspis*; He, *Hemicyclaspis*; Ho, *Hoelaspis*; Ki, *Kiaeraspis*; Sp, *Spatulaspis*; St, *Stensiopelta*;
263 Tr, *Tremataspis*. See also Table S1.

264

265 **STAR METHODS**

266

267 **RESOURCE AVAILABILITY**

268 **Lead contact**

269 Further information and requests for resources should be directed to and will be fulfilled by
270 the Lead Contact, Humberto G. Ferron (Humberto.Ferron@bristol.ac.uk).

271

272 **Materials Availability Statement**

273 This study did not generate new unique reagents.

274

275 **Data and code availability**

276 The datasets generated during this study are available at the Bristol Research Data Facility
277 (<https://data.bris.ac.uk/data/dataset/1bjnv53uzx5dm2nw0q2tdtbqji>).

278

279 **EXPERIMENTAL MODEL AND SUBJECT DETAILS**

280 **Geometric morphometric analysis**

281 We limited our study to species of established taxa and conducted analyses at generic level,
282 with each genus represented by a single specimen. We used the type species and holotype
283 specimen for each genus except where this specimen was poorly preserved; in such cases,
284 another well-defined species was used instead. We included a total of 30 specimens in the
285 analysis, some of which exhibited minor deformation due to dorso-ventral compression
286 (Table S2). This deformation was not corrected for due to the difficulties in doing so without
287 introducing additional sources of error; previous work has demonstrated that biological signal
288 is still retained when deformation is minor [40]. Images of specimens for digitization were
289 obtained from photographs or published reconstructions (Data S2).

290

291 **METHOD DETAILS**

292 **Geometric morphometric analysis**

293 The morphological diversity of osteostracan headshields was summarized and numerically
294 described using geometric morphometrics, following the procedure detailed in Ferrón et al.
295 [41]. We digitized a total of 123 landmarks of type I, II and III on selected images using TpsDig
296 v.2.26 [42] (Figure 1b). Type III landmarks were equally interpolated along the specimen
297 outline in six different open curves. The number of Type III landmarks chosen to represent
298 each curve was determined visually, reflecting the complexity and relative length of each part
299 of the headshield. Variation in translation, rotation and size from the original landmark
300 configurations was removed by generalized Procrustes analysis (GPA) in MorphoJ v. 1.06d
301 [43] without implementing sliding methods for Type III landmarks. This choice is fully justified
302 as sliding and non-sliding semilandmark methods provide similar superimpositions and PCA
303 morphospaces (Figure S1 and Table S3) [44]. Distance matrices were obtained considering
304 Euclidean distances and subjected to principal coordinate analysis in the packages ‘cluster’

305 [45] and 'ape' [46] in R [47]. Morphospaces and phylomorphospaces were constructed using
306 the R packages 'Phytools' [48] and 'ggplot2' [49] based on pre-ordination ancestral state
307 estimation [50]. Ancestral state reconstruction was achieved through stochastic character
308 state mapping [51] using the R package 'geomorph' [52]. This analysis was based on the
309 phylogenetic relationships proposed by Samson [53], after modification in Mesquite [54] and
310 time-calibration in the R package 'paleotree' [55], according to the stratigraphic ranges
311 published by Samson et al [56] (Data S3).

312

313 **Three-dimensional virtual modelling**

314 Eight species of osteostracans ("*Boreaspis*" *ceratops*, *Cephalaspis lyelli*, *Hemicyclaspis*
315 *murchisoni*, *Hoelaspis angulata*, *Kiaeraspis auchenaspidoides*, *Spatulaspis robusta*,
316 *Stensiopelta pustulata* and *Tremataspis schmidtii*), covering a good representation of all
317 occupied regions of the morphospace (Figure 1c), were modelled virtually using 3D Studio
318 Max (Data S4). Digital models obtained by three-dimensional virtual modelling have been
319 shown to be reliable tools to assess function through computational analysis, providing very
320 similar results to those derived from tomographic or surface-based techniques [57]. Here,
321 modelling was based on photographs of fossil specimens and/or published reconstructions in
322 multiple views (Table S4; see also Table S2 for a list of the specimens studied first hand).
323 Complete headshields of all selected species are known and are usually preserved as three-
324 dimensional structures, ensuring the accuracy of reconstructions. The postcranial region was
325 accurately modelled for taxa in which it is known (i.e., *Cephalaspis* [58], *Hemicyclaspis* [59]
326 and *Tremataspis* [60]), whereas a generalized osteostracan morphology was used for the
327 remaining species. Spinal processes were represented on the dorsal line of the *Stensiopelta*
328 model because these structures are known to be present in other zenaspidid osteostracans

329 [18]. Pectoral fins were modelled as paddle-like structures [61,62] and were positioned
330 according to the location of the area of attachment. Digital reconstructions were scaled to life
331 size using Netfabb Basic and converted into NURBS surface using Geomagic Studio.

332

333 **Computational fluid dynamics analyses**

334 Simulations of water flow around the three-dimensional osteostracan models were
335 performed using COMSOL Multiphysics 5.2 (www.comsol.com). Two different computational
336 domains were used to emulate pelagic and benthic conditions. For the pelagic scenario, the
337 computational domain consisted of a three-dimensional cylinder (1500 mm in length and 300
338 mm in diameter) in which the osteostracan model was centrally fixed and positioned at eight
339 different angles of attack (0° to 70° , every 10°) (Figure 1d). For the benthic scenario, the
340 computational domain consisted of a three-dimensional half-cylinder (1500 mm in length and
341 300 mm in diameter) in which the osteostracan model was fixed at 0.1, 0.5 and 1.0 body
342 lengths above the lower surface of the domain (Figure 1d). We evaluated the domain size to
343 confirm it was sufficiently large that it did not influence fluid flow (Data S1).

344

345 An inlet with a normal inflow velocity boundary condition with a turbulence intensity of 0.05
346 was defined at one end of the domain, and an outlet with a zero pressure boundary condition
347 was specified at the opposing end. Boundaries at the top and sides of the domain were “open”
348 (slip boundary condition), approximating flow through the domain, whereas the boundaries
349 at the water–fossil interface were “solid” (no-slip boundary condition), fixing the fluid velocity
350 at zero. The flat lower boundary of the half-cylinder used only in the benthic scenario was
351 assigned a “moving wall” boundary condition, given the same velocity as the inlet. In all cases,
352 an automatic wall treatment was used, with surface roughness not specified. The domain was

353 meshed using free tetrahedral elements and the ‘normal’ mesh size parameter in COMSOL
 354 Multiphysics. To determine the influence of mesh size on the results of the CFD simulations,
 355 we used three different meshes in an initial exploration of mesh quality for the *Kiaeraspis* and
 356 *Stensiopelta* models, corresponding to the smallest and largest species, respectively. We
 357 evaluated ‘coarser’ (maximum element size of 78.0 mm and minimum element size of 24.0
 358 mm), ‘coarse’ (maximum element size of 60.0 mm and minimum element size of 18.0 mm),
 359 and ‘normal’ (maximum element size of 40.2 mm and minimum element size of 12.0 mm)
 360 meshes. In all cases, smaller elements were used in regions close to the fossil. Drag and lift
 361 results obtained from normal and coarse meshes are very similar (see table below). As a result,
 362 we selected a ‘normal’ mesh for use in our study because increasing the mesh quality further
 363 would necessitate a large increase in computation time without any improvement in accuracy.
 364 An inlet velocity of 0.3 m s⁻¹ was considered in all the cases.

365

366 *Kiaeraspis* (pelagic scenario, angle of attack 40°):

Mesh	Drag force (N)	Drag coefficient	Lift force (N)	Lift coefficient
Coarser	0.00689	0.51105	0.00758	0.56289
Coarse	0.00708	0.52508	0.00797	0.59177
Normal	0.00696	0.51669	0.00801	0.59467

367

368 *Stensiopelta* (pelagic scenario, angle of attack 40°):

Mesh	Drag force (N)	Drag coefficient	Lift force (N)	Lift coefficient
Coarser	0.10126	0.52276	0.09647	0.49802
Coarse	0.10719	0.55337	0.10427	0.5383
Normal	0.10808	0.55797	0.10267	0.53004

369

370 Three-dimensional, incompressible flow was simulated through the domain, with a stationary
 371 solver used to compute the steady-state flow patterns. A realistic ambient flow velocity [63]

372 of 0.30 m s^{-1} was simulated (Reynolds numbers of 17100 to 64500). The Reynolds averaged
373 Navier-Stokes (RANS) equations were solved using the shear stress transport (SST) turbulence
374 model and a segregated solver algorithm; segregated iterations terminated when the relative
375 tolerance (0.001) exceeded the relative error, computed as the minimum of the solution-
376 based error and the error given by the Residual factor (1000) times the residual-based error.
377 The effect of increasing inlet velocity was tested in parallel by simulating inlet velocities of
378 0.65 and 1.00 m s^{-1} (Reynolds numbers of 37050 to 215000; Table S1).

379

380 The results were visualized as plots of pressure (Pa) over the surface of the osteostracan
381 models. Drag and lift forces and their coefficients (C_D and C_L) were calculated to quantify the
382 flow around the digital reconstructions. For this, the headshield area was taken as the
383 reference area. Apparent weight of each taxon was also calculated for comparative purposes
384 assuming a body density of 1100 kg m^{-3} [64]. This value is in agreement with previous
385 estimations on other ostracoderms considering the distribution and density of dermal bone,
386 soft tissues and internal cavities [65]. All COMSOL Multiphysics files containing the
387 simulations are available in the Bristol Research Data Facility
388 (<https://data.bris.ac.uk/data/dataset/1bjnv53uzx5dm2nw0q2tdtbqji>).

389

390 **QUANTIFICATION AND STATISTICAL ANALYSIS**

391 Phylogenetic generalized least square (PGLS) analysis was undertaken in MorphoJ v. 1.06d
392 [43] to test for correlations between shape changes and C_D and C_L . These analyses were
393 performed for one benthic (0.1_{BL}) and three pelagic (at 0° , 10° and 20°) scenarios, which were
394 considered the most biologically realistic conditions. In all cases, we considered 0.05 as the
395 level of statistical significance.

396

397 **SUPPLEMENTAL INFORMATION FILE LEGENDS**

398 **Data S1. Sensitivity analysis of domain size. Related to STAR Methods.**

399 **Data S2. Images used for the geometric morphometric analysis. Related to STAR Methods.**

400 **Data S3. R code and files used in the construction of the phylomorphospaces. Related to**
401 **STAR Methods.**

402 **Data S4. Three-dimensional models used for the computational fluid dynamics analyses.**
403 **Related to STAR Methods.**

404 **Table S1. Results of all CFD analyses performed for the eight selected species of**
405 **osteostracans including details of how the Reynolds number, apparent weight, and the drag**
406 **and lift coefficients and lift-to-drag ratios were calculated. Related to Figure 3.**

407

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