

1 Brain enlargement and dental reduction were not linked in hominin evolution

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14

15 Abstract

16 The large brain and small postcanine teeth of modern humans are among our most
17 distinctive features, and trends in their evolution are well studied within the hominin
18 clade. Classic accounts hypothesize that larger brains and smaller teeth co-evolved
19 because behavioral changes associated with increased brain size allowed for a
20 subsequent dental reduction. However, recent studies have found mismatches between
21 trends in brain enlargement and posterior tooth size reduction in some hominin species.
22 We use a multiple variance Brownian motion approach in association with evolutionary
23 simulations to measure the tempo and mode of the evolution of endocranial and dental
24 size and shape within the hominin clade. We show that hominin postcanine teeth have
25 evolved at a relatively consistent neutral rate, whereas brain size evolved at

26 comparatively more heterogeneous rates that cannot be explained by a neutral model,
27 with rapid pulses in the branches leading to later *Homo* species. Brain reorganization
28 only shows evidence of elevated rates much later in hominin evolution, suggesting that
29 fast-evolving traits, such as the acquisition of a globular shape, may be the result of
30 direct or indirect selection for functional or structural traits typical of modern humans.

31

32 **Keywords**

33 Endocast, postcanine teeth, evolutionary rates, selection, paleoanthropology

34

35 **Significance statement**

36 The evolution of posterior teeth and brains seems to follow parallel trends in hominins.
37 Larger brain size is associated with reduced premolar and molar crowns, but this
38 association is not observed in all hominin species. We have evaluated this association in
39 a quantitative way by measuring lineage-specific rates of dental and cerebral evolution
40 in the different branches of the hominin evolutionary tree. Our results show that
41 different species evolved at different rates, and that brain evolution in early *Homo* was
42 faster than dental evolution. This result points to different ecological and behavioral
43 factors influencing the evolution of hominin teeth and brains.

44

45 /body

46

47 **Introduction**

48

49 The large brains and small posterior teeth of modern humans are among our most
50 distinctive features, and trends in their evolution are well studied because of the

51 phylogenetic and functional implications of variation in dental and cerebral anatomy (1-
52 3). Brain expansion and postcanine reduction appear to follow parallel trends during
53 hominin evolution and classic views consider that an increase in brain size was linked to
54 a more complex behavior that included the manufacture and use of stone tools, which
55 allowed for a subsequent dental reduction. A shift towards a higher-quality diet during
56 the evolution of early *Homo* has also been related to brain size increase and posterior
57 tooth reduction (4, 5). However, it has recently been suggested that in early *Homo* brain
58 expansion—as inferred from endocranial capacity—substantially preceded dental
59 reduction (6). It has also been noted that early in the Neanderthal lineage dental
60 reduction preceded the additional brain expansion seen in the later ‘classic’
61 Neanderthals (7). The suggestion that stone tool use and manufacture substantially
62 predated the increase in brain size observed in early *Homo* (8) adds further complexity
63 to this scenario.

64

65 Recent developments in ancestral state reconstruction (9, 10) allow lineage-specific
66 patterns of brain expansion and dental reduction to be quantified and compared. Unlike
67 traditional approaches to ancestral state reconstruction that assume a neutral
68 evolutionary scenario, which is likely unrealistic in most cases, we used a variable rate
69 approach that estimates differences in evolutionary rates across different branches of a
70 given phylogeny. We applied this approach to quantitative data on endocranial and
71 postcanine dental size and shape in order to develop a comprehensive scenario of trends
72 in endocranial and dental evolution across the hominin clade (Fig. 1). Our assessment
73 used a framework phylogeny based on widely agreed evolutionary relationships and on
74 the currently estimated first and last appearance dates for eight of the most broadly
75 accepted hominin species (11) (Fig. 1, Table S1). Amounts of change along each branch

76 of the hominin phylogenetic tree estimated through the variable rate approach were
77 compared with the amount of change observed in evolutionary simulations that used a
78 constant variance Brownian motion (BM) model (12) in which traits evolve neutrally
79 and at a constant rate, without directional trends in any particular branch of the hominin
80 phylogeny (Methods).

81

82 **Results**

83 Among the four traits, endocranial volume is the only one whose evolution has given
84 rise to patterns of variation that are significantly different from those obtained from
85 neutral simulations (Fig. S1). The standard deviation of the amounts of change per
86 branch observed across the phylogeny is significantly greater than the standard
87 deviations obtained in constant-rate simulations of the evolution of endocranial size
88 ($P=0.017$). This indicates that lineage-specific patterns of brain size evolution are more
89 heterogeneous than expected under a neutral model and unlikely to be explained by
90 genetic drift. In addition, the rates of change for endocranial and dental size and shape
91 through time differ substantially in different parts of the hominin phylogeny (Figs. 2
92 and 3). These differences are robust to different sample composition ($P<0.001$ for all the
93 pairwise comparisons between the four traits) and to corrections for small sample size
94 (Fig. S2), and they are substantial for most branches of the hominin phylogeny (Table
95 S2, Fig. S3). Although we use the term *rate* to make reference to branch-specific
96 amounts of change, it should be noted that these values are not rates in the strict sense
97 because they do not represent amounts of change per unit of time, but the ratio of
98 observed to simulated change per branch (see Methods).

99

100 Our results show that sustained rapid evolution in brain size started before the
101 separation of *Paranthropus* and *Homo*, and peaked before the divergence between *H.*
102 *erectus* and the lineage leading to Neanderthals and modern humans (Fig. 3A). That
103 peak rate was more than 4 times greater than that observed in simulated neutral
104 scenarios (Table S2). Additional rapid brain increase was observed in the lineage
105 immediately predating the Neanderthal-modern human split, but this was only twice as
106 fast as that observed in a neutral scenario (Table S2). Other branches within the hominin
107 phylogeny show much slower rates of change than those observed in a pure BM
108 process, which is consistent with stabilizing selection and constrained evolution. These
109 estimates are similar to the ones obtained when using a more traditional approach to
110 quantify branch-specific change based on a generalized least squares (GLS) ancestral
111 reconstruction method (Table S3), which detects fast and slow evolutionary rates in the
112 same branches, but with less extreme values.

113

114 Our results support the long-standing hypothesis that within the hominin clade brain
115 organization, as inferred from endocranial shape, evolved independently of brain size
116 (13). The ratios between the endocranial shape change measured along each branch and
117 those simulated using BM were all close to 1, leading to a general scenario that is not
118 statistically different from those observed in constant-rate simulations ($P=0.355$, Fig.
119 S1). This indicates that endocranial shape evolved according to a quasi-neutral model,
120 which is consistent with a scenario where genetic drift is predominant (Fig. 3B). Rapid
121 change, about twice that expected under a BM model, was observed only along the
122 branch leading to modern humans from their last common ancestor with Neanderthals
123 (Table S2). This rapid evolutionary change is reflected in the principal component
124 analysis of endocranial shape variation, which shows that *H. sapiens* strongly diverges

125 from all other species along PC1 (Fig. 2B). The eigenvector of this axis shows that the
126 dorsal arc connecting the frontal and occipital poles is the only variable loading
127 positively on PC1, thus separating flatter from the more globular endocasts that
128 distinguish *H. sapiens* (14-16) (Table S4). Researchers have suggested that
129 globularization is driven by upper parietal reorganization, and that this anatomical
130 change can be associated with enhanced visuospatial integration and memory in modern
131 humans (17). The comparatively fast evolution of the dorsal arc trait in the lineage
132 leading to *H. sapiens* is consistent with such a link between brain anatomy and function,
133 although it could be an indirect result of selection on other craniofacial hard-tissue
134 changes (18). If some individuals that do not show a globular anatomy, such as Jebel
135 Irhoud 1 and 2, and Omo 2, are early members of *H. sapiens* (19), then the endocranial
136 anatomy typical of modern humans may have evolved within the *H. sapiens* lineage.

137

138 Although there are differences in branch-specific evolutionary rates for dental size, they
139 are still within the expectations of a constant-rate model ($P=0.257$, Fig. S1). Sustained
140 reduction in the posterior dentition began in the branches antedating the origin of the
141 genus *Homo* and continued along the sequence of branches leading to *H. sapiens* (Figs.
142 2C and 3C). Dental reduction along all these branches occurred at a rate that was
143 approximately twice as fast as expected under a neutral evolutionary model (Table S2).
144 Although the size of posterior teeth of *H. habilis* and *A. afarensis* is similar, a fast
145 evolutionary rate is inferred before the evolution of early *Homo* because this change is
146 calculated with respect to the last common ancestor of *Paranthropus* and *Homo*, which
147 is inferred to have had larger posterior teeth than *A. afarensis* (Fig. 2C). A rapid rate of
148 dental reduction continued on the lineage leading to modern humans, but not in
149 Neanderthals, resulting in the comparatively small postcanine dentition of our species

150 [Fig. 2C, ref. (20)]. A previous quantitative study of molar size found that molar
151 reduction observed in *H. erectus*, Neanderthals and modern humans occurred at a faster
152 rate than in early *Homo* (21). That study, however, used M2 area as a proxy for molar
153 size without considering variation in molar proportions across the molar row. Those
154 proportions are known to change in the genus *Homo* in concert with absolute molar size,
155 thus making M2s and M3s disproportionately small in species with overall small dental
156 size (22, 23). Reduction in the dentition was not the only rapidly evolving trend because
157 dental expansion occurred at similarly high rates in the lineage leading to *Paranthropus*
158 species (Fig. 2C, Table S2). Our data suggest that posterior tooth size in *P. robustus*
159 stabilized after its divergence from the *P. boisei* lineage, whereas *P. boisei* continued its
160 dental expansion, but in a way consistent with quasi-neutral evolution. Assuming that
161 the *Paranthropus* clade is monophyletic, which is the most common assumption even if
162 other explanations are possible (24), these observations suggest that *Paranthropus*
163 postcanine megadontia is the result of long term selective pressures that predate the
164 divergence of the *Paranthropus* species.

165

166 As with endocranial shape, the shape of tooth crowns also evolved under a quasi-neutral
167 model in which the evolutionary change along each branch is close to and statistically
168 indistinguishable from that expected from a pure BM model ($P=0.528$, Fig. 3D, Fig.
169 S1). The difference that drives the first principal component of dental crown shape is a
170 preferential reduction of the distal areas of premolars and molars in Neanderthals and
171 modern humans (Fig. 2D; Fig. S4). The most rapid evolutionary change on the tree (1.5
172 times greater than that expected in a neutral scenario) is associated with this change
173 along the branch antedating the separation of Neanderthals and modern humans (Table
174 S2). Although both species share strong reduction of the distal regions of posterior

175 teeth, they have their own species-specific configurations. The characteristically derived
176 dentition of Neanderthals (25, 26) is reflected in the relatively fast rate of evolution of
177 dental shape in this lineage (Table S2).

178

179 **Discussion**

180 Our results show clear differences in evolutionary patterns corresponding to endocranial
181 and dental size and shape during hominin evolution. Endocranial volume evolved at
182 relatively heterogeneous rates that differ significantly from those observed under a
183 constant-rate neutral model (Fig. S1). Endocranial shape and dental size and shape
184 evolved at comparatively more uniform rates, with shape traits evolving under a quasi-
185 neutral model. Although the evolution of these traits does not significantly differ from
186 the expectations of a constant-rate scenario, endocranial shape, dental size and dental
187 shape still show significantly different evolutionary patterns. Given similar genetic
188 variance, drift is expected to affect all traits in the same population equally (27). Studies
189 of brain anatomy in chimpanzees and modern humans, however, have shown that brain
190 size and brain organization have substantially different heritabilities (28), which
191 represent the proportion of total phenotypic variance in a population that has a genetic
192 basis. Therefore, genetic variances of the traits included in our study can plausibly be
193 different, which might explain their different evolutionary behavior even if neither
194 significantly differs from neutrality.

195

196 The observed patterns of branch-specific variation are consistent regardless of sample
197 size and composition (Fig. S2), but they could be affected by changes in the
198 phylogenetic scenario. We have chosen to deal with phylogenetic uncertainty by
199 removing from our analyses those species whose phylogenetic position is particularly

200 controversial, such as *H. ergaster*, *H. antecessor* and *H. heidelbergensis*. The resulting
201 phylogenetic topology generally agrees with most quantitative and qualitative
202 assessment of hominin phylogenetic relationships (21, 29, 30), but new fossil findings
203 resulting in different relationships or branch lengths could potentially modify some of
204 our findings.

205

206 Our results, which indicate that the evolution of hominin brain organization and brain
207 size are decoupled, are consistent with larger brain size being positively selected across
208 the entire genus *Homo* (31). Strong selection for larger brains has been linked to the
209 selective advantages associated with the enhanced computational abilities of a larger
210 neocortex with more neurons (32), but it can be also linked to other neural
211 modifications such as an increased developmental plasticity arising from changes in the
212 developmental patterns associated with larger brains (28, 33, 34). Selection for certain
213 aspects of brain organization, particularly in the upper parietal reorganization that is
214 arguably associated with modern human-specific functional modifications (17), is
215 confined primarily to the branch leading directly to *H. sapiens*. No other aspects of
216 brain reorganization as described by our set of variables show evidence of fast evolution
217 across the hominin clade. However, many aspects of brain reorganization are not
218 captured by those endocranial metrics, particularly those related to finer-grained
219 organization such as sulcal variation and brain asymmetries, among others. The
220 predominant role of neutral mechanisms in the evolution of endocranial shape is
221 consistent with previously published work reporting a major role of genetic drift in
222 craniofacial evolution during the *Australopithecus-Homo* transition (35, 36) and during
223 the divergence of Neanderthals and modern humans (37). Although our study focuses

224 on endocranial variation, our findings are consistent with a general neutral scenario for
225 the evolution of craniofacial shape in hominins.

226

227 The evolution of tooth crown size and shape are more closely linked than are the
228 evolution of brain size and shape. The branch antedating the separation of Neanderthals
229 and modern humans is characterized by strong reduction in overall dental size
230 associated with strong localized reduction of the distal area of the crown of all
231 postcanine teeth (20, 26). This anatomical change, however, took place over a long
232 period of time and does not show evidence of particularly fast evolution indicating
233 strong selection. Although *H. sapiens* shows substantially faster reduction in dental size
234 than Neanderthals, the two species share similar evolutionary rates of crown shape
235 evolution, thus demonstrating that their species-specific dental traits have been subject
236 to similar selection intensities. Crown shape evolution does not radically depart from a
237 Brownian motion model and most branches within the hominin phylogeny have evolved
238 at very similar rates with respect to postcanine dental shape. This observation lends
239 quantitative support to dental shape as a useful proxy for reconstructing phylogenetic
240 relationships in hominin fossil species. Indeed, the utility of dental shape to infer
241 evolutionary relationships is also supported by recent DNA analyses of Middle
242 Pleistocene European fossils (38, 39), which have confirmed their relationship with
243 Neanderthals, as it was initially proposed using fossil evidence (7, 26).

244

245 If branch-specific trends are not quantified, the sustained brain expansion found in some
246 of the branches of the genus *Homo* may appear to be associated with sustained dental
247 reduction. However, our results, which show that teeth and brains evolved at different
248 rates in different hominin species, suggest that the two trends were “decoupled”. Our

249 analysis shows that the apparent coupling of the traits is confined to the three branches
250 that connect the last common ancestor of *Paranthropus* and *Homo* with the last
251 common ancestor of Neanderthals and modern humans and that, even in those cases,
252 brain evolution occurred at faster rates. We suggest that the context-specific ecological
253 and behavioral factors that influenced the evolution of teeth and brains were not the
254 same for the two morphological regions, nor were the combinations of those factors the
255 same at different stages during hominin evolution.

256

257 **Materials and methods**

258 **Materials** We used four datasets to evaluate postcanine and endocranial size and shape
259 (Table S1, Datasets 1-4). The dental size and shape dataset was assembled by one of us
260 (AGR) as part of quantitative descriptions of occlusal postcanine morphology (26, 40).
261 Those samples were pruned to include only species with relatively uncontroversial
262 phylogenetic positions (see below), and for which data on endocranial size and shape
263 were also available. Endocranial size was studied using species-specific endocranial
264 volumes based on values listed in ref. (41). This data set does not reflect the reduction
265 in endocranial volume seen in recent *Homo sapiens*. Mean cranial capacity in *Homo*
266 *erectus* was estimated from a subsample of Asian *Homo erectus* that shares a similar
267 geographical and chronological origin as the dental sample (41). Endocranial shape was
268 evaluated in a smaller sample of complete or partial hominin endocasts.

269

270 **Quantitative description of dental and endocranial size and shape** Postcanine dental
271 shape was characterized with configurations of landmarks and sliding semilandmarks
272 on the occlusal surface of tooth crowns (26, 40) and dental size was quantified as the
273 centroid size of those configurations (defined as the square root of the sum of the

274 squared distances between each landmark and the center of gravity of the
275 configuration). Procrustes superimposition (42) was used to remove variation in
276 position, size, and orientation, and species-specific mean shapes were obtained by
277 averaging Procrustes-superimposed coordinates for each species (26). Principal
278 components analyses of Procrustes coordinates were used to obtain the principal
279 component (PC) scores used in subsequent analyses (12). When all dimensions of shape
280 variation are considered, which we did throughout all our analyses, PC scores contain
281 the same information as original variables, but they are mathematically more convenient
282 (12).

283

284 The size and shape data were pooled to analyze the complete postcanine dentition. For
285 shape analyses, landmark coordinates corresponding to the ten postcanine teeth (upper
286 and lower premolars and molars) were subjected to different Procrustes
287 superimpositions, and were then combined in the same principal components analyses.
288 Overall dental size was estimated by summing up centroid sizes across all the
289 postcanine teeth. Analyses of dental size, therefore, reflect increases or decreases of
290 total postcanine occlusal areas, but not changes in dental proportions among teeth.

291

292 Endocranial size was evaluated using species-specific mean endocranial volumes.
293 Endocranial shape was quantified using a set of classic linear metrics measured by
294 RLH. These metrics included eight variables used in other studies of hominin
295 endocranial variation (Fig. 1, ref. 43). Size variation was removed from these analyses
296 by dividing each of these metrics by the cube root of cranial capacity in each individual.
297 Species-specific mean values for each of these variables were subjected to principal

298 components analysis, and PC scores were used in ancestral reconstructions of
299 endocranial shape.

300

301 The robustness of our results to sample composition was evaluated by bootstrapping the
302 original samples 1,000 times, and then recalculating species-specific mean values and
303 running all the analyses in bootstrapped samples. Likewise, we assessed if the more
304 heterogeneous evolutionary rates obtained for endocranial evolution with respect to
305 dental evolution result from differences in sample size. Because some of the species in
306 our samples are represented by only 3 endocasts, we jackknifed all the samples to three
307 individuals per species. This down-sampling process was also repeated 1,000 times.
308 Resampling rounds for both approaches were performed independently for each tooth
309 position because most individuals in the dental samples do not preserve all postcanine
310 teeth.

311

312 **Hominin phylogeny** Because our methodological approach requires the use of an *a*
313 *priori* phylogeny, we used only species whose phylogenetic positions are relatively
314 uncontroversial. Following the most widely accepted view, we considered *Homo* and
315 *Paranthropus* as two monophyletic clades (29) [but see ref. (44)]. *A. africanus* was
316 considered to be a sister group to both *Paranthropus* and *Homo* clades following ref.
317 (45), although some analyses have suggested other phylogenetic positions for this
318 species (29), including a recent classification as a sister group only to *Homo* (30). We
319 chose not to use a pruned version of the recently published Bayesian phylogeny
320 proposed in ref. (30) for two reasons. Firstly, the supermatrix on which this analysis is
321 based pools traits and character states based on different studies, criteria and scoring
322 systems, which may bias results by recovering nodes that have little or no support or by

323 failing to recover nodes that do have high support (46). Secondly, posterior probabilities
324 yielded by this analysis for most of the nodes included in our phylogeny are very low.
325 Although unquestionably valuable for considering alternative scenarios for hominin
326 evolution, we believe that evolutionary relationships reflected in the summary of best
327 trees presented in ref. (30) have in general weaker support than the relationships used in
328 our study.

329

330 Times of node divergence and ages of terminal species followed ref. (11). Tips were
331 dated to the last appearance date (LAD) for each species listed in Table 1 of ref. (11),
332 whereas nodes were dated to the corresponding first appearance date (FAD). Assuming
333 that FADs and LADs observed in the fossil record are unlikely to represent the actual
334 FADs and LADs for each species, we used the non-conservative version of these dates,
335 which incorporate "the age, and the published error of the age, of the nearest underlying
336 dated horizon in the case of the FAD, and the age, and the published error of the age, of
337 the nearest overlying dated horizon in the case of the LAD" [ref. (11), p. 55].

338

339 To account for some phylogenetic patterns that are not reflected in these values, we
340 dated the oldest ancestor in our tree to 4.4 Ma assuming an evolutionary continuity
341 between *A. anamensis* and *A. afarensis* (47), which was dated to 2.9 Ma. The
342 divergence between *P. robustus* and *P. boisei* was established at 2.3 Ma. To account for
343 the recent early *Homo* findings that have pushed back the FAD of the genus *Homo* to at
344 least 2.8 Ma (48), we set the origin of this genus at 2.9 Ma. The divergence of the
345 *Paranthropus* and *Homo* clades was estimated at 3.5 Ma. Because our samples do not
346 include late *H. erectus* fossils, we dated *H. erectus* to 400 ka. An early Neanderthal
347 status for Sima de los Huesos hominins is strongly supported by both the

348 paleontological and molecular evidence (7, 38, 49), so we established the divergence
349 date of Neanderthals and modern humans at 0.5 Ma, although morphological studies
350 suggest that an earlier divergence time for these species is likely (26, 30). The averaging
351 of data points at the last appearance dates used for each species is likely to provide
352 conservative estimates of branch-specific amounts of change. However, the use of data
353 at time points that are closer to individual values would artificially inflate the measured
354 amounts of change per branch due to the uncertainty regarding finer-grained population-
355 specific dates and their particular relationships.

356

357 **Ancestral estimation** A multiple variance Brownian motion (mvBM) framework was
358 used to estimate ancestral values in the hominin phylogeny (10). Most ancestral
359 estimation approaches assume a standard Brownian motion model of character
360 evolution (BM) (50). In standard BM the rate of evolution is assumed to have a single
361 mean and variance across all branches, and trait divergence is proportional to the square
362 root of time. Biologically, these assumptions imply there is no sustained difference in
363 the direction and rate of change among the different lineages of the phylogeny. In many
364 cases we expect this assumption to be unrealistic because selection may be associated
365 with environments that differ systematically between subclades or with particular
366 evolutionary or environmental events that occurred on only one branch of the tree, thus
367 producing different evolutionary rates and directions in different lineages. Our approach
368 relaxes the pure BM model in order to capture different patterns of trait variation along
369 each branch of the phylogeny (10).

370

371 Specifically, ancestral values were estimated using a two-step process. The first step
372 infers branch-specific patterns of change based on a model that assumes that trait values

373 for ancestral nodes are a compromise between global and local effects. The baseline
374 assumption that phylogenetic relatedness accurately reflects how traits evolve is hereby
375 leveraged against local deviations from this expectation. Specifically, a ‘global’
376 estimate (a weighted estimate based on the phylogenetic tree and the tip values) is
377 combined with a ‘local’ estimate (accounting for information from a node’s closest
378 relatives without taking tree structure into account) in order to accurately capture
379 lineage-specific changes that may deviate from the baseline expectation that
380 phylogenetic relatedness provides an accurate proxy of how traits evolve. Measures of
381 the rate of evolution are then estimated by dividing the squared trait difference by the
382 branch length for each ancestor-descendant pair. Rates hereby represent the extent to
383 which lineage-specific changes are found to align with the baseline expectation that
384 phylogenetic relatedness is an accurate proxy for trait evolution. Each branch rate can
385 be considered to be a point estimate of the rate of change along each individual branch
386 under a multiple variance BM model.

387

388 In the second step, the branch lengths of the original phylogenetic tree are rescaled
389 according to the estimated rates of evolution in order to account for branch-specific
390 differences from the baseline expectation that phylogenetic relatedness only is an
391 accurate proxy of trait evolution. The model with the rescaled branches is then
392 parameterized using a standard BM model in order to produce ancestral estimates. This
393 procedure makes use of the analytical power of BM estimation techniques while
394 allowing for local variation in evolutionary rates. This method—which is explained in
395 greater detail in ref. (10) and implemented in the R package 'evomap' (51)—was
396 applied to the hominin phylogeny and endocranial and dental datasets.

397

398 **Evolutionary simulations** Results obtained through the previously described process
399 were compared with results obtained through a simulated pure BM scenario. For size
400 traits, evolutionary variation was simulated on log-transformed size values, whereas for
401 shape variation, PC scores were used (12). Simulations were initiated at the ancestral-
402 most values estimated through the mvBM approach. A per-generation variance rate
403 (per-generation σ^2) was estimated after rescaling the hominin phylogeny to generations
404 using a constant generation time of 25 years (52). A generalized least squares approach
405 (53) implemented in the package 'Phylogenetics' for *Mathematica* (54) was used to
406 estimate a constant per-generation variance rate for each variable (log-size and PC
407 scores) based on available data.

408

409 Using trait-specific constant per generation rates, evolutionary change was simulated as
410 a uni- or multidimensional random walk (12) on the hominin phylogeny. Simulations
411 were run 1,000 times and the mean change between all ancestors and descendants was
412 used as the expectation of the amount of change if each branch had evolved neutrally
413 under a pure BM model. For endocranial and dental shape, this simulation was
414 performed in PC morphospace. Shape distances between ancestors and descendants
415 were calculated as the square root of the sum of the squared differences in all PC scores
416 between two given species, which is equivalent to the definition of Procrustes distance
417 for landmark data. For dental and endocranial size, branch-specific amounts of change
418 were calculated simply as the difference between descendants and ancestors.

419 Transformations between landmark coordinates and PC morphospace were done with
420 the package 'Geometric Morphometrics' for *Mathematica* (55).

421

422 The mvBM branch-specific changes were compared to the pure BM changes as the ratio
423 mvBM/BM. A value larger than 1 indicates that a given branch has experienced more
424 change than expected under a BM model (that is, that branch has evolved faster than
425 expected under a neutral model regardless of the directionality of the change). A value
426 smaller than 1 is indicative of slower evolution than that expected under a neutral
427 model, which is in turn indicative of stabilizing selection along a certain branch. As we
428 emphasized earlier, although we refer to these values as *rates*, we recognize that they
429 are not rates in the strict sense, but the ratio of observed to simulated change per branch.
430 These values were color coded and overlaid on the original phylogeny.

431

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440

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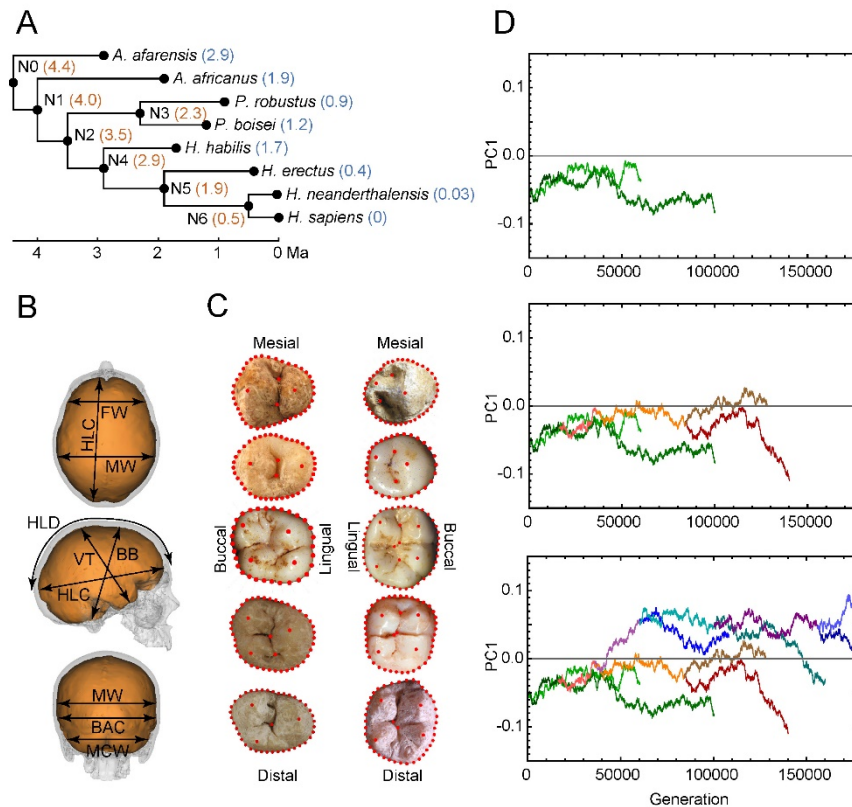
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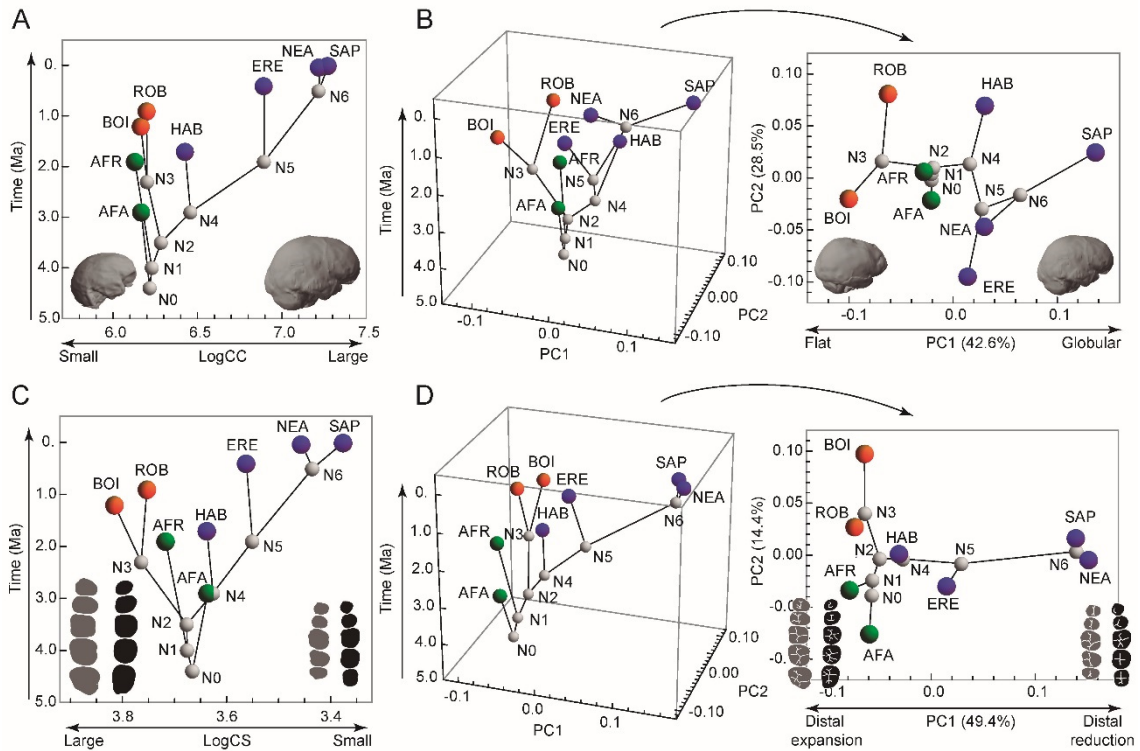
581 **Fig. 1. Methodological setup of the study.** (A) Hominin phylogeny employed in our
 582 analyses, indicating the dates used for terminal species (blue) and nodes (orange). (B)
 583 Linear metrics used in the study of endocranial variation. FW: frontal width at Broca's
 584 cap; HLC: hemispheric length chord; MW: maximum endocranial width; HLD:
 585 hemispheric length dorsal arch; BB: basion-bregma distance; VT: vertex-lowest
 586 temporal distance; BAC: biasterionic chord; MCW: maximum cerebellar width. (C)
 587 Landmark and semilandmark datasets used in the study of postcanine dental variation.
 588 Upper teeth are on the left and lower teeth on the right. Postcanine teeth are represented
 589 from top to bottom following the sequence P3, P4, M1, M2 and M3. (D) Brownian
 590 motion simulation of the evolution of one trait (PC1 score) across the hominin
 591 phylogeny. Top: green shading shows evolution along the *A. afarensis* and *A. africanus*
 592 branches. Middle: simulated evolution along the *Paranthropus* clade is added in orange-
 593 red shading to the above plot. Bottom: simulated evolution along the *Homo* clade is

594 added as blue shading to the above graph. B and C have been modified after refs. (26,

595 43).

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597



598

599 **Fig. 2. Variation in endocranial and dental size and shape through time. (A)**

600 Change in endocranial size (logarithm of cranial capacity) over time showing extreme

601 examples of variation. (B) Principal components analysis of endocranial shape variation

602 over time is shown on the left, and the projection of PC1 and PC2 without time is

603 represented on the right. (C) Change in dental size (logarithm of centroid size) over

604 time. (D) Principal components analysis of dental shape variation over time (left), and

605 without time (right). In A and B, the small and flat endocasts are the *A. afarensis* Sts 5

606 and *P. robustus* SK 1585 specimens. The large and globular endocast is a recent *H.*

607 *sapiens*. Endocasts are in the same orientation as in Figure 1. In C and D dental

608 silhouettes representing large and distally expanded dentitions are based on the *P.*

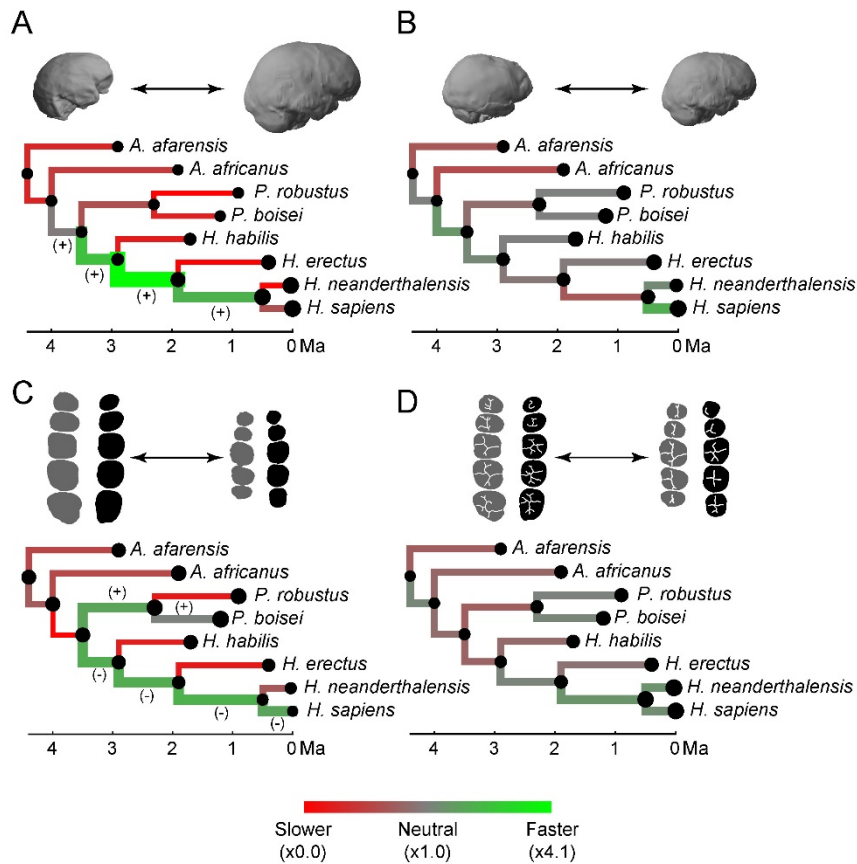
609 *robustus* specimens SK 13/14 (upper teeth) and SK 23 (lower teeth). Small and distally

610 reduced dentitions are based on a recent *H. sapiens*. Orientation of teeth is the same as

611 in Figure 1. AFA: *A. afarensis*; AFR: *A. africanus*; ROB: *P. robustus*; BOI: *P. boisei*;

612 HAB: *H. habilis*; ERE: *H. erectus*; NEA; *H. neanderthalensis*; SAP: *H. sapiens*.

613



614

615 **Fig. 3. Evolution of endocranial and dental size and shape.** (A) Comparison of
 616 observed and simulated branch-specific amounts of endocranial size variation. (B)
 617 Comparison of observed and simulated amounts of endocranial shape variation. (C)
 618 Comparison of observed and simulated amounts of dental size variation. (D)
 619 Comparison of observed and simulated amounts of dental shape variation. Red
 620 represents stasis along a given branch and green represents fast evolution along a given
 621 branch, regardless of the directionality of change. Branch thickness is proportional to
 622 the observed amount of change along a given branch. In A and C, (+) represents size
 623 increase and (-) represents size decrease along fast-evolving branches, and tip and node
 624 size is proportional to endocranial and dental size. In B and D the amount of change per
 625 branch is based on shape distances that include all dimensions of the morphospace, and
 626 node and tip size is proportional to the amount of shape change with respect to the

627 ancestral-most node. Example specimens are the same as in Figure 2. Orientation of

628 endocasts and teeth is the same as in Figures 1 and 2.

629