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2 **Geometric morphometrics and Finite elements analysis: Assessing the functional**  
3 **implications of differences in craniofacial form in the hominin fossil record**

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26 **Abstract:**

27 The study of morphological variation in the hominin fossil record has been transformed in  
28 recent years by the advent of high resolution 3D imaging combined with improved geometric  
29 morphometric (GM) toolkits. In parallel, increasing numbers of studies have applied finite  
30 elements analysis (FEA) to the study of skeletal mechanics in fossil and extant hominoid  
31 material. While FEA studies of fossils are becoming ever more popular they are constrained  
32 by the difficulties of reconstruction and by the uncertainty that inevitably attaches to the  
33 estimation of forces and material properties. Adding to these modelling difficulties it is still  
34 unclear how FEA analyses should best deal with species variation.

35 Comparative studies of skeletal form and function can be further advanced by applying tools  
36 from the GM toolkit to the inputs and outputs of FEA studies. First they facilitate virtual  
37 reconstruction of damaged material and can be used to rapidly create 3D models of skeletal  
38 structures. Second, GM methods allow variation to be accounted for in FEA by warping  
39 models to represent mean and extreme forms of interest. Third, GM methods can be applied  
40 to compare FEA outputs – the ways in which skeletal elements deform when loaded. Model  
41 comparisons are hampered by differences in material properties, forces and size among  
42 models but how deformations from FEA are impacted by these parameters is increasingly  
43 well understood, allowing them to be taken into account in comparing FEA outputs.

44 In this paper we review recent advances in the application of GM in relation to FEA studies  
45 of craniofacial form in hominins, providing examples from our recent work and a critical  
46 appraisal of the state of the art.

47

48 **Keywords:** Form-function; Geometric Morphometrics; Finite Element Analysis; Craniofacial  
49 form; Functional performance.

50

51

## 52 **1. Introduction**

53 In this paper we consider how the mechanical performance of crania in biting can be  
54 estimated and compared among fossils, paying particular attention to how the methods of  
55 geometric morphometrics (GM) can facilitate such analyses in combination with  
56 biomechanical modelling using finite elements analysis (FEA).

57

58 As with other skeletal elements, crania fulfil mechanical functions, such as housing and  
59 protection of organs and provision of a rigid framework for food acquisition and intra-oral  
60 processing by the masticatory apparatus (Lieberman, 2011), which comprises jaws, teeth and  
61 soft tissues. Thus, much research has focused on the association between cranial form and  
62 masticatory function, with the aims of understanding how crania function and how their  
63 functional abilities (performances) differ among related species. These differences have  
64 underpinned investigations of how skeletal form, function, ecology and behaviour interrelate  
65 (Groning, et al., 2011b, Rayfield, 2005, Rayfield, 2007, Rayfield, et al., 2001, Strait, et al.,  
66 2010, Strait, et al., 2007, Strait, et al., 2009, Wroe, et al., 2010, Wroe, et al., 2007). In turn,  
67 knowledge of these interrelationships has been used to infer ecology and behaviour from  
68 skeletal remains of extinct taxa (Attard, et al., 2014, Cox, et al., 2015, Degrange, et al., 2010,  
69 Ledogar, et al., 2016, Oldfield, et al., 2012, Rayfield, 2005, Rayfield, et al., 2001, Smith, et  
70 al., 2015b, Strait, et al., 2010, Strait, et al., 2009, Wroe, 2008).

71

72 One aspect of performance, bite force, can be directly measured in extant species using force  
73 transducers. These have been widely used to measure bite forces in living humans (Braun, et  
74 al., 1995, Kikuchi, et al., 1997, Paphangkorakit and Osborn, 1997, Sinn, et al., 1996). In  
75 extinct material alternative approaches are required to estimate forces from skeletal evidence,  
76 using bony proxies to approximate lever arm lengths and maximum muscle forces based on  
77 the relationships between muscle area, intrinsic muscle fibre strength and force production  
78 (Gans and de Vree, 1987, Josephson, 1975, Weijs, 1980). Although this provides an estimate  
79 of the force produced by muscles it ignores pennation and depends on the validity of the  
80 estimates of muscle areas from bony proxies. Muscle force is converted into bite force  
81 through the masticatory lever arm system. By measuring in and out-levers of the masticatory  
82 system and computing their ratios, it is possible to estimate the mechanical efficiencies of  
83 each muscle and to estimate maximal bite forces (Antón, 1990, Demes and Creel, 1988, Eng,

84 et al., 2013, O'Connor, et al., 2005). However, this approach has limitations due to  
85 differences between the cross sectional areas estimated via bony proxies and actual  
86 physiological muscle cross sectional areas (Eng, et al., 2013, Toro-Ibacache, et al., 2015), and  
87 because the lever system of the jaws is often simplified to two dimensions to ease  
88 calculations. Bite force can also be predicted using FEA (Wroe, et al., 2010) and by  
89 multibody dynamic analysis (MDA) (Bates and Falkingham, 2012, Curtis, et al., 2008, Shi, et  
90 al., 2012). MDA can also be used to infer muscle activation patterns given a particular load.  
91 These approaches take full account of the three dimensional geometry of the masticatory  
92 lever system but retain dependence on the accuracy of input of variables, such as muscle  
93 forces, force vector directions and cranial geometry.

94 Bite forces are transmitted to items held between the teeth, and the teeth and cranium  
95 experience the bite reaction force. Thus, crania have to be adapted to withstand masticatory  
96 forces. In order to assess, explain and compare how the cranium resists occlusal forces,  
97 researchers have used several approaches. These include the analysis of simplified  
98 biomechanical models of craniofacial anatomy considered in terms of vertical and horizontal  
99 column-like structures that buttress the face and channel bite reaction forces (Görke, 1904;  
100 Richter, 1920; Endo, 1965; Endo, 1966) and models that consider crania as a cylinder that is  
101 twisted during biting (Greaves, 1985; Greaves and Mucci, 1997; Demes, 1987). These  
102 models and their underlying assumptions have been tested through the application of strain  
103 gauges to directly measure the surface strains experienced during biting (Hylander et al.,  
104 1991; Hylander et al., 1992; Ross and Hylander, 1996; Ravosa et al., 2000a; Ravosa et al.,  
105 2000b; Ross, 2001; Ross et al., 2011). FEA has also been applied to this task (Ledogar, et al.,  
106 2016, Smith, et al., 2015b, Strait, et al., 2010, Strait, et al., 2007, Strait, et al., 2009, Wroe, et  
107 al., 2010) but an important issue in such studies is validity of FEA results, do they match  
108 reality?

109

110 For this reason validation studies have been carried out to assess the accuracy of prediction of  
111 cranial and mandibular deformations, comparing measured with predicted strains (Bright and  
112 Groning, 2011, Groning, et al., 2009, Kupczik, et al., 2007, Ross, 2005, Toro-Ibacache, et al.,  
113 2016). In so doing, researchers can assess how various input parameters including skeletal  
114 geometry, material properties, constraints, applied forces etc. impact FE model results in  
115 order to create more realistic models (Ross, 2005, Strait, et al., 2005, Toro-Ibacache, et al.,  
116 2016). In general validation studies tell us that accurate strain prediction in any one specimen  
117 is difficult and requires careful adjustment of model parameters to achieve valid results.

118

119 The accuracy of predictions achieved by FEA is, however, entirely dependent on these input  
120 parameters, so, acknowledging modelling limitations, researchers have sought to understand  
121 the impact of variations and simplifications in FE modelling. This has led to sensitivity  
122 studies in which the impact on predicted deformations of varying specific parameters is  
123 assessed. Such parameters include the muscle force magnitudes, directions and activation  
124 patterns (Cox, et al., 2011, Fitton, et al., 2012, Groning, et al., 2012, Ross, 2005, Sellers and  
125 Crompton, 2004), variations in material properties (Cox, et al., 2011, Groning, et al., 2012,  
126 Kupczik, et al., 2007, Reed, et al., 2011, Strait, et al., 2005, Toro-Ibacache, et al., 2016),  
127 modelling cranial sutures (Kupczik, et al., 2007, Reed, et al., 2011, Wang, et al., 2010),  
128 simplifications in model geometry (Fitton, et al., 2015, Toro-Ibacache, et al., 2016),  
129 modelling the periodontal ligament (Groning, et al., 2012, Holland, 2013, McCormack, et al.,  
130 2014, Wood, et al., 2011), impact of variations in modelling of trabecular bone (Parr, et al.,  
131 2013) and model constraints (Cox, et al., 2011). Validation and sensitivity studies have  
132 shown that modelling variations that affect model stiffness (e.g. bone thicknesses, how  
133 cancellous bone is represented, material properties, etc.) or total applied force tend to lead to  
134 differences in magnitude rather than mode of deformation, while variations in relative muscle  
135 activations, muscle vectors and constraints tend to impact mode of deformation, how the  
136 cranium deforms (Fitton, et al., 2015, Godinho, et al., 2017, Parr, et al., 2012, Toro-Ibacache,  
137 et al., 2016).

138

139 Researchers have tried to predict how fossil hominin crania resist biting. Such analyses have  
140 until recently relied on geometrical simplifications of crania (Demes, 1987, Rak, 1983, Rak,  
141 1986, Trinkaus, 1987). More recently, FEA has been used to more fully model fossil hominin  
142 masticatory biomechanics with the aim of improving prediction of the stresses and strains  
143 experienced by fossil crania as they deform during biting (Ledogar, et al., 2016, Smith, et al.,  
144 2015b, Strait, et al., 2010, Strait, et al., 2009, Wroe, et al., 2010). Sensitivity studies are of  
145 particular relevance here as validation is not possible for fossils. FEA applied to fossils has  
146 become popular (Cox, et al., 2011, Cox, et al., 2012, Rayfield, 2007, Strait, et al., 2013,  
147 Strait, et al., 2010, Strait, et al., 2007, Strait, et al., 2009, Wroe, et al., 2010, Wroe, et al.,  
148 2007) and models are frequently based on medical CT scans. However, another challenge of  
149 fossils arises because they are often fragmented and invaded by sedimentary matrix that, due  
150 to mineralization processes, is undistinguishable, or at least very difficult to distinguish, from  
151 bone in scans. This often precludes, for example, segmentation of sedimentary matrix from

152 bone and does not allow fossils to be modelled reliably in terms of their full anatomical  
153 complexity. Indeed, given the multiscale organisation of bone, teeth and soft tissues, it is not  
154 within the reach of present technology to produce an accurately realistic model. Moreover,  
155 increasing model complexity demands higher computational power for solution (Groning, et  
156 al., 2012).

157

158 Model simplification in geometry is therefore useful and necessary to overcome these  
159 limitations (Fitton, et al., 2015). Assessment of the impact of simplifications typically relies  
160 on comparison of variables of interest in subsequent FEA. Thus, researchers commonly focus  
161 on stress/strain magnitudes and directions and compare how different modelling decisions  
162 impact on those variables (Groning, et al., 2012, Reed, et al., 2011, Strait, et al., 2005,  
163 Szwedowski, et al., 2011, Wood, et al., 2011), although bite force has also been used to  
164 assess model sensitivity (Fitton, et al., 2012, Sellers and Crompton, 2004). Beyond this, the  
165 methods of geometric morphometrics have recently been applied to this task; to compare the  
166 deformations of variant models and estimate the impact of such simplifications on results  
167 (Fitton, et al., 2015, Fitton, et al., 2012, Godinho, et al., 2017, Toro-Ibacache, et al., 2016).

168

169 The application of GM methods to FEA output is discussed below in more detail, as it is  
170 used for the reconstruction of fossils for FEA and in the creation of models of interesting real  
171 and hypothetical forms.

172

## 173 **2. How GM can help in reconstruction**

174 Once the segmentation process is finished, reconstruction of missing anatomical regions  
175 begins. This process usually combines imaging software (e.g.  
176 Avizo/Amira/Mimics/Geomagic) and GM to approximately restore the original geometry of  
177 an incomplete or distorted specimen (Weber, 2015, Weber and Bookstein, 2011). In  
178 specimens that preserve one side intact, the most straightforward approach is to use bilateral  
179 symmetry (Gunz, et al., 2009). In such cases it is possible to reflect the preserved regions  
180 onto the incomplete side and use them to replace the missing areas (Gunz, et al., 2009).  
181 However, no skeletal structures are completely symmetric and they present different  
182 magnitudes of asymmetry (Quinto-Sánchez, et al., 2015). Thus, reflected regions will not  
183 perfectly fit the remaining preserved anatomy. To overcome this mismatch, and account for  
184 asymmetry, it is possible to use the thin plate spline (TPS) function to warp the reflected



185 structure onto the remaining preserved anatomy (Gunz, et al., 2009). Even though this is a  
186 desirable approach, fossils often lack preserved structures on both sides or along the midline,  
187 thus precluding reflection. In these cases reference based reconstruction (Gunz, et al., 2004,  
188 Gunz, et al., 2009) should be used. The choice of reference specimen should be considered  
189 carefully so as to not bias the reconstruction and it has been suggested that references should  
190 be species specific (Gunz, et al., 2009, Senck, et al., 2015, Zollikofer and Ponce de León,  
191 2005). Such reconstructions may be statistical or geometric (Gunz, et al., 2004, Gunz, et al.,  
192 2009, Neeser, et al., 2009). Statistical reconstruction uses covariances among landmarks in a  
193 given sample to predict the location of missing landmarks via multivariate regression (Gunz,  
194 et al., 2009, Neeser, et al., 2009). Geometric reconstruction uses the TPS function to estimate  
195 the position of the missing landmarks based on known ones (Gunz, et al., 2004, Gunz, et al.,  
196 2009). The latter has the advantage of requiring one single specimen, which may be a  
197 particular individual or a mean specimen calculated from a given sample using GM (Gunz, et  
198 al., 2009) but omits information on intra specific covariations. However, Senck and  
199 Coquerelle (2015) show that using mean specimens yields good results when reconstructing  
200 large portions of incomplete specimens. Further where sample sizes are limited to one or a  
201 few specimens, as with fossils, TPS based warping can be applied, whereas statistical  
202 approaches cannot.

203

### 204 **3. How GM can generate interesting hypothetical forms**

205 Transforming an existing model into a target specimen is of significant value in allowing us  
206 to visualise the results of GM analyses. To that end an original specimen may be landmarked  
207 densely and then warped into a target that was landmarked similarly (O'Higgins, et al., 2011,  
208 Stayton, 2009). Models that represent extremes of morphological variation within a taxon  
209 may be created applying a similar approach. Such models can readily be used to simulate  
210 mechanical loading and examine the impact of intra-specific morphological variance on  
211 mechanical function (Smith, et al., 2015a). One major obstacle to using such an approach is  
212 that accurate warping of one specimen into another requires many landmarks and  
213 semilandmarks and even then, internal structures such as tooth roots, sinuses and cancellous  
214 bone are unlikely to be warped to the form they would have in the target specimen. This is  
215 because such internal architecture is very finely detailed and sinuses and cancellous bone  
216 architecture are, to great extent, the result of adaptation in the specific individual to habitual  
217 loading, this is not accounted for by warping alone. Any errors in warping will therefore

218 likely impact the resulting deformations of the FE model. An alternative is to warp ‘solid’  
219 models, ones in which all that is represented is the geometry of the cranial surfaces with the  
220 spaces in between infilled with homogenous material. Cancellous bone and sinuses are filled  
221 and teeth are not represented as distinct structures, but merely as material with the properties  
222 of bone, and with roots merged with the surrounding bone. This is a drastic manoeuvre and a  
223 gross simplification. As such, the question arises as to what solid simplified models can tell  
224 us?

225

226 Parr et al. (2012) examined the impact of infilling mandibular cavities on the deformations  
227 (bending displacements and strain magnitudes frequency) experienced by the mandible of a  
228 varanoid lizard during simulated loading. They show that models with infilled cavities  
229 deform less than, but generally similarly to, models with preserved cavities. Likewise, Fitton  
230 et al. (2015) investigated the effects of simplifying details of internal anatomy  
231 (presence/absence of the maxillary sinus) and material properties of teeth in a *Macaca*  
232 *fascicularis* cranium, concluding that it does not impact significantly on large scale  
233 deformations but it does have localized effects in strain distributions. Toro-Ibacache (2016)  
234 addressed the impact of segmentation protocols and of simplifying material properties of a  
235 cadaveric human cranium. They concluded that segmentation protocols can have a significant  
236 impact on large scale deformations but that simplifying material properties (differentiating  
237 trabecular bone from cortical bone vs not differentiating between the two) had little impact on  
238 mode of deformation. Thus, if constraints and loads are held constant, solid models behave  
239 similarly to much more detailed ones. The key difference emerging from these studies is that  
240 the solid models deform less, and so absolute magnitudes of deformation (measured as strains  
241 or in terms of changes in size and shape; see below) are not accurately predicted while the  
242 mode of deformation (how it deforms) is more consistent. This leads to the realisation that  
243 solid models are useful in studies where absolute magnitudes of strains are of no interest but  
244 rather, the focus is on mode, how a cranium deforms.

245

246 These findings open up the possibility of carrying out many interesting ‘virtual experiments’  
247 by warping or modifying skeletal anatomy to predict the functional role of particular features  
248 (O’Higgins, et al., 2011). Strait et al. (2007) applied this virtual experiment approach to infer  
249 the relevance of thick palates in Australopiths by experimentally thickening the hard palate of  
250 a *Macaca fascicularis* and measure resulting strains. Fitton et al. (2009) reconstructed a  
251 specimen of *Australopithecus africanus* (STS 5) and warped the zygomatic region to that of a

252 *Paranthropus boisei* (OH 5) while maintaining the remaining anatomy constant. In both  
253 cases, the impact of such modifications was assessed in terms of their impact on stresses and  
254 strains in the face.

255

#### 256 **4. How GM can be used to compare FEA results**

257 While stresses and strains from FEA are informative with regard to how skeletal structures  
258 bear loads and where they are likely to fail at a localized level (elements or nodes of  
259 elements) they do not allow ready assessment of how the model deforms as a whole, for  
260 instance, how it bends, twists and undergoes other changes in size and shape. Rather, such  
261 modes have to be inferred from strain contour maps based on expertise and knowledge.

262 GM, on the other hand, uses configurations of landmark coordinates and multivariate  
263 statistics to assess how specimens differ in form, thereby quantifying morphological  
264 differences in size and shape. Thus, it has been proposed that GM can be used to measure and  
265 describe global deformations (defined here as changes in size and shape) of models under  
266 loading (O'Higgins, et al., 2011, O'Higgins, et al., 2012). This approach differs from GM  
267 shape analyses in that size is also simultaneously considered, because loadings change the  
268 shape and the size of objects. The basis and application of this approach is described more  
269 fully in section 5.3.

270

#### 271 **5. Example Studies**

272 To illustrate how the approaches described above are applied in practice, example studies are  
273 presented and reviewed, below.

274

##### 275 **5.1 Reconstruction of crania**

276 We illustrate the application of GM to reconstruction using a CT scan of the cranium of  
277 Kabwe 1, which is remarkably well preserved but still presents missing and damaged  
278 anatomy due to taphonomic and pathological processes (Schwartz and Tattersall, 2003).  
279 Missing anatomical regions include a large portion of the right side of the cranial vault and  
280 base (affecting parts of the right temporal, parietal, zygomatic and occipital bone), a small  
281 region of the alveolus of the maxilla, teeth and small portions of the orbital cavities (Figure  
282 1A). The reconstruction was based on a CT scan (courtesy of Robert Kruszynski, Natural

283 History Museum, London) performed using a Siemens Somatom Plus 4 CT scanner, with  
284 voxel size of 0.47 x 0.47 x 0.50 mm and 140 kVp. Reconstruction started with the  
285 segmentation of the existing anatomy from the volume. Reconstruction of the left side of the  
286 vault followed, and this was later used to restore the large region missing from the right side  
287 of the cranium. Lastly, all remaining missing anatomical regions were reconstructed.  
288 Segmentation was performed in Avizo 7.0 (Visualization Sciences Group Inc.) and used a  
289 variety of approaches. The initial segmentation applied a half maximum height value  
290 (HMHV; Spoor et al., 1993) to the whole volume to threshold segment it. Regional  
291 thresholds were subsequently calculated and applied to specific anatomical regions as a  
292 second step because the HMHV did not segment thin bones. Manual segmentation was also  
293 applied for fine details of thin bones that were not picked up by the two previous approaches.  
294 Because teeth present clearly different grey values specific thresholds were calculated and  
295 applied so as to not overestimate their dimensions. Last, existing sedimentary matrix was  
296 removed manually.

297

298 Once the segmentation of existing structures was complete, the large missing region of the  
299 right half of the cranium was restored by reflecting the existing contralateral half and fitting  
300 (warping) it to the existing structures. This last step used the TPS function and is necessary  
301 because crania are not absolutely symmetric. This warping is achieved by placing matching  
302 landmarks on the damaged region and reflected fragment and then deforming (warping) the  
303 fragment to the cranium using the 'Bookstein' warping function. This resulted in an almost  
304 perfect fit between the restored and preserved anatomy, requiring only minimal manual  
305 editing. Restoration of the damaged alveolar process of the right hemi-maxilla was also  
306 achieved by reflecting the preserved left region. Existing gaps (such as the one present in the  
307 orbital surfaces of the maxilla and ethmoid, internal nasal walls, maxilla, occipital bone, left  
308 temporal bone, ethmoid bone and vomer) were restored using a combination of manual  
309 editing and the software Geomagic Studio 2011 (courtesy of DR W. Sellers, University of  
310 Manchester) to interpolate between existing bone edges. The missing posterior region of the  
311 occipital bone was reconstructed using the occipital of a modern human cranium, which was  
312 manually edited using Geomagic to adjust its morphology. Teeth were preferentially restored  
313 by reflecting existing antimeres. When this was not possible portions of teeth from a modern  
314 human were used to reconstruct incomplete teeth (final result of reconstruction in Figure 1B).

315

316

317 Figure 1

318

319

## 320 **5.2 Hypothetical forms**

321 FEA may be applied to any model, whether it represents a real specimen or not. For instance  
322 a prior GM analysis may have established the mean form and limits of variation of a  
323 landmark configuration taken on a sample of crania. Rather than be interested in how any  
324 particular specimens perform, we may be interested in the range of performances represented  
325 by the sample. Earlier we noted that solid models, in which internal detail is grossly  
326 simplified and filled, provide a reasonable basis for experimental manipulation of FE models  
327 to assess specific questions such as the effects of varying palatal thickness or maxillary  
328 morphology. This same principle can be extended to whole landmark configurations such as  
329 those representing the limits of variation of a sample. By using triplets of thin plate splines to  
330 warp whole crania between the mean and these limits of variation hypothetical crania can be  
331 created. They do not represent real crania but rather a statistical result from prior  
332 morphometric analyses, in this case limits of variation but also, feasibly, through regression  
333 or partial least squares (PLS), they could represent forms at the limits of cranial covariation  
334 with some interesting ecological or functional variables (e.g. climatic or dietary data,  
335 measured bite forces etc.). FEA is then carried out on these hypothetical forms to see how the  
336 modes of variation of cranial form identified in the analysis impact performance when the  
337 cranium is loaded.

338

339 This warping approach is illustrated here using a simple example; the Kabwe 1 cranium  
340 warped into a mean Neanderthal (model 2) using thin plate splines based on classical and  
341 sliding semi-landmarks. Classical landmarks (Figure 2, red spheres) of the mean Neanderthal  
342 were calculated from 4 Neanderthal crania (Gibraltar 1, Guattari, La Chapelle-aux-Saints, La  
343 Ferrassie). The sliding semi-landmarks on the maxilla and brow-ridge (yellow spheres) were  
344 calculated from the 4 specimens and the sliding semi-landmarks of the vault and zygoma  
345 (light blue spheres) were calculated from the 2 crania in which these structures are almost  
346 completely preserved (Guattari and La Ferrassie). In Figure 2, the original model of Kabwe is  
347 shown on the left (Figure 2A) and the warped 'mean Neanderthal' on the right (Figure 2B). It  
348 is clear that a visually satisfactory result is obtained but of course internal architecture (tooth

349 roots, cortical thicknesses, cavities, sinuses and cancellous bone) will also be warped, not  
350 necessarily in such a way that they reasonably represent the average form in Neanderthals.  
351 However, by using ‘solid’ models as described above such errors are avoided. The FEA in  
352 such a circumstance does not aim to predict and compare actual deformations but rather it  
353 provides an answer to a different type of question: how do the differences in external form  
354 between these models impact mode and magnitude of deformation?

355 This approach is more limited than we may wish but it is useful in many contexts, for  
356 instance in considering how facial retraction vs projection, or brachycephaly vs  
357 dolichocephaly, or the mode of form variation predicted by e.g. climate or diet etc. impact on  
358 model performance. These are more general questions whose answer does not rest on study  
359 of single specimens, but rather on consideration of general modes of variation and their  
360 general effects.

361

362

363 Figure 2

364

365

### 366 **5.3 Application of GM methods to the comparison of FEA results**

367 As noted earlier a third way in which GM methods complement FEA is through comparison  
368 of deformations that occur due to loading (O'Higgins, et al., 2011, O'Higgins, et al., 2012).  
369 This approach has been applied in several studies (Cox, et al., 2011, Fitton, et al., 2015,  
370 Groning, et al., 2012, Groning, et al., 2011a, Holland, 2013, Prôa, 2013, Toro-Ibacache, et al.,  
371 2016). Such analyses of deformation rely on assessment of changes in model size and shape,  
372 rather than of shape alone as is common in GM studies of organismal variation. This is  
373 because as a model is loaded it changes in both size and shape, and it makes no sense to focus  
374 on one aspect alone (shape or size). In consequence size and shape are analysed jointly, using  
375 rescaled shape coordinates from GPA. The resulting size and shape distances between  
376 unloaded and loaded forms describe the magnitudes of deformation and the direction of the  
377 vector connecting unloaded and loaded forms in the size and shape space describes the mode  
378 of deformation. These vectors can be compared among different load cases applied to the  
379 same model or among different models by ignoring the differences in size and shape among  
380 unloaded forms and focussing in the vectors connecting unloaded and loaded forms.

381 We illustrate the application of this approach by summarizing a study (Godinho, et al., 2017,  
382 Toro-Ibacache, et al., 2016) that examines the impact of simplifications of a cadaveric *Homo*  
383 *sapiens* cranium on the resulting modes of deformation predicted by FEA. Specifically, it  
384 assesses the impact of simplifications among a three materials model (cortical bone,  
385 cancellous bone and teeth; model 3), a two materials (cortical bone and teeth; model 2) and a  
386 one material model (everything with material properties of cortical bone; model 1). Thus  
387 model 1 is a simple 'solid' model (see above) and model 3 is a much more anatomically  
388 accurate model. The models are loaded to simulate a bite on the first molar, although the  
389 applied forces are not physiological, rather they replicate the loading of an accompanying  
390 validation study to facilitate comparison with that in ongoing work.

391 The results in terms of strain contour plots (not shown), suggest that variations among models  
392 generally impact on magnitudes of strains but not so much on the distribution of regions of  
393 high and low strain throughout the model. The GM analysis of deformations complements  
394 these findings. Size and shape distances are calculated by multiplying the shape coordinates  
395 (from GPA) of each specimen by that specimen's original centroid size. This results in the  
396 specimens being represented by points in a (size and shape) space that can be thought of as  
397 the space of GPA aligned coordinates (Slice 2001), an approximation of Kendall's shape  
398 space, with size as an additional dimension. The vector of centroid size (the additional  
399 dimension) at any point on the manifold can be visualised as passing radially from the  
400 centroid of the manifold of this space (zero size), through the manifold (centroid size = 1) and  
401 beyond to infinity (infinite size). When centroid size is 1, the objects lie on the manifold of  
402 the space of GPA aligned coordinates (Figure 3). The resulting space differs from the classic  
403 size and shape space (Dryden and Mardia, 1998) that results from translating and rotating, but  
404 not scaling landmark configurations. In particular, the rotations of configurations with respect  
405 to each other differ because size influences rotation. In consequence the estimates of mean  
406 size and shape (the size and shape variables; translated and rotated coordinates) obtained by  
407 these two approaches, the resulting covariance matrix, and so PCA, also differ. However in  
408 the application to FEA, where deformations are extremely small, the resulting size and shape  
409 differences are negligible. Either space could be used, with almost no difference in results,  
410 but the approach we adopt is useful in understanding how shape analysis and size and shape  
411 analysis are related (Figure 3). Thus, simply making the model stiffer or less stiff (material  
412 properties) or applying the same force vectors but varying their magnitudes results in greater  
413 or less deformation; the vectors connecting unloaded and loaded models simply scale directly  
414 with force or inversely with Young's modulus (a measure of stiffness). Deformations (size

415 and shape distances) also scale inversely with model centroid size if loads, geometry and  
416 material properties are held constant. In contrast Procrustes distances scale inversely with the  
417 square of centroid size. Figure 3 illustrates these scaling relationships with centroid size.  
418 Thus if we take the shape of the black point (a; on the GPA hemisphere, centroid size =1;  
419 Fig. 3) to be the unloaded form and the grey point (b) as the shape of the loaded form, the  
420 distance between them represents the deformation in shape and approximates Procrustes  
421 distance when variations are small. If size also differs due to loading, then the loaded form  
422 does not lie on the hemisphere but is above (grey point, c) or below it depending on if it  
423 increased or decreased in centroid size. The distance (a-c) between loaded and unloaded  
424 forms is the size and shape distance and is a measure of deformation (change in size and  
425 shape with loading).

426

427 If the same forces and same material properties apply but the unloaded form is larger (black  
428 point, d, on the outer semicircle representing the GPA hemisphere with centroid size >1 in  
429 Fig 3) the resulting deformation in size and shape is less (distance d-f; which in this diagram  
430 is shown larger than in reality to facilitate visualisation). The physics dictate that the size and  
431 shape distances (deformations) between unloaded and loaded objects scale inversely with  
432 centroid sizes of the unloaded objects; bigger forms deform less under the same load.  
433 However, shape change due to loading (Procrustes distance as opposed to size and shape  
434 distance) scales inversely with the *square* of the centroid size of the unloaded object. Thus,  
435 scaling the unloaded large object, d, to centroid size 1, results in it overlying point a, the  
436 unloaded object with centroid size 1 (these are identical in shape but differ only in size).  
437 Scaling the loaded large object, f, to centroid size 1 projects it along a radius (dashed line in  
438 Fig. 3) through point e to an intersection, g, with the arc of the GPA hemisphere. As a result  
439 of this scaling, the ratio of Procrustes distances (a-b)/(a-g) is the inverse of the ratio of the  
440 squares of centroid sizes of the unloaded forms, a and d.

441

442 These scaling ratios are important because they allow us to account (at least approximately)  
443 for differences in size when comparing deformations predicted by FEA among similar objects  
444 using geometric morphometric methods. Such scaling is inevitably an approximation unless  
445 the objects whose deformations are being compared are the same shape, differing only in  
446 size. As shapes become more different, it makes less sense to compare deformations and the  
447 degree of approximation in scaling increases.

448



449 Figure 3

450

451

452 Principal components analysis using the covariance matrix among size and shape variables  
453 can be used to visualise and compare deformations. Figure 4 presents the first two principal  
454 components from the sensitivity study we conducted on a *Homo sapiens* of model  
455 simplification with regard to segmentation and allocation of material properties. These  
456 account for some 99% of the total variance and so fairly represent the results. Included in the  
457 analysis are the unloaded model and the three variants of model segmentation (model 1,  
458 whole model as cortical bone = 17 GPa; model 2, bone = 17 GPa and teeth = 50 GPa; model  
459 3, cortical bone = 17GPa, cancellous bone = 56 MPa, teeth = 50 GPa; all materials allocated a  
460 Poisson's ratio of 0.3) after loading in a simulated first molar bite. Model 3 is also loaded in a  
461 simulated incisor bite. This allows the effects of simplification to be compared against the  
462 effect of varying bite point. The molar bites cluster away from the incisor bite, indicating  
463 they are more similar in mode of deformation. The modes of variation are represented by the  
464 vectors connecting unloaded and loaded models. They are visualised by the inset warped  
465 surface models and transformation grids, computed using thin plate splines and magnified  
466 500 times to facilitate interpretation. Models 2 and 1 overlies each other and so are represented  
467 by a single point. This implies that representing dental roots as cortical bone has little effect.  
468 Modes of deformation differ greatly between incisor and molar bites and consist mainly of  
469 upwards deflection of the anterior maxilla in the former and of the lateral maxilla in the latter.  
470 With regard to the molar bites, simplification has its greatest impact when cancellous bone is  
471 allocated the material properties of cortical, effectively making a 'solid' model. The effect is  
472 to reduce the degree of deformation as is reflected in the shorter vector connecting models 1  
473 and 2 with the unloaded than that connecting model 3. Similarly the degree of deformation  
474 evident in the inset warpings is reduced. There is a difference in mode of deformation as  
475 evidenced by the angle between these vectors but the difference in mode is less obvious in  
476 comparing the inset warping for models 2 and 3 with that for model 1.

477 The impact of simplification on mode of deformation is small compared to the large  
478 difference between molar and incisor bites.

479

480

481 Figure 4

482

483

484 This simple analysis can be extended to more complex and interesting questions concerning  
485 multiple variants of models and to the comparison of deformations among models (O'Higgins  
486 and Milne, 2013) by focusing on differences among vectors of deformation rather than  
487 differences among unloaded forms. This application of GM is particular useful in relation to  
488 FEA sensitivity studies providing an easily visible and quantifiable approach to the  
489 assessment of model “error” and sensitivity. Comparisons can be made within and between  
490 models to assess whether differences in performance due to modelling assumptions are  
491 drowning out any meaningful biological signals.

492

## 493 **6. Discussion**

494 The last three decades have seen an explosion of advances in techniques pertinent to the  
495 study of skeletal change through time. Morphometrics underwent a revolution (Adams, et al.,  
496 2004, Rohlf and Marcus, 1993) beginning in the late 1970's (Bookstein, 1978) and gathering  
497 pace through the next three decades. This, in common with the tools for high resolution  
498 imaging, visualisation and manipulation of images, took great advantage of the advances in  
499 computing that occurred over the same period. These same advances in computational power  
500 led to the development of increasingly sophisticated software tools for FEA, to simulate and  
501 predict the effects of loadings on structures.

502

503 All of these tools are in common use today in the field of Archaeology, in particular they  
504 have been driven by work on fossil material, but increasingly they are applied to more recent  
505 skeletal finds, archaeobotany (García-Granero, et al., 2016, Ros, et al., 2014), zooarchaeology  
506 (Cucchi, et al., 2011, Evin, et al., 2013, Owen, et al., 2014) and to material culture such as  
507 ancient architecture (Levy and Dawson, 2009), stone tools (Buchanan and Collard, 2010,  
508 Buchanan, et al., 2011, Okumura and Araujo, 2014), and pottery (Hein, et al., 2008,  
509 Kilikoglou and Vekinis, 2002, Wilczek, et al., 2014). As these tools have become more  
510 commonly applied, useful ways of combining them have come to the fore. Thus, GM  
511 methods combined with tools for imaging and image manipulation can play an important role  
512 in the reconstruction of skeletal material, as illustrated by the first example we present in this  
513 paper.

514

515 Reconstruction provides data for morphometric analyses and GM has proven powerful in this  
516 domain. Beyond the fact that these methods provide approaches that are statistically robust  
517 and well understood, GM's great advantage for many workers lies in the ability to visualise  
518 the results of statistical analyses as warpings of the mean form. These visualisations close the  
519 loop between measurement, statistics and interpretation of results in terms of changes in size  
520 and shape. They also can be used to produce 3D models of the results of statistical analyses  
521 such as mean forms or forms representing extremes of variation or extremes of interesting  
522 modes of variation, such as the limits of regressions of form on ecological, behavioural and  
523 functional data. In turn, such forms are potentially interesting targets for FEA. For instance,  
524 the results of a study of how cranial form covaries with the toughness of diet might be  
525 actualised as a pair of 3D surfaces representing crania at the limits of the regression; those  
526 suited to tough and those suited to less tough diets. These can be submitted to FEA to explore  
527 how each responds to loading and, in this way, link modes of morphological variation to load  
528 resistance. This kind of analysis provides a very direct way of exploring how form and  
529 function interact.

530

531 These kinds of studies depend critically on the validity of FEA modelling and on how  
532 sensitive such modelling is to errors in model building and loading. Validity is assessed by  
533 comparing predicted strains with directly measured, real strains. Sensitivity, on the other  
534 hand is assessed by varying model parameters to replicate likely errors and comparing results  
535 among (often many) variant models as in the example we provide earlier. In this endeavour,  
536 GM has been usefully combined with FEA.

537

538 Size and shape analysis allows ready understanding of the effects of different model building  
539 decisions in terms of how the models deform and how they differ in deformation. It leads to  
540 statements about changes in form such as how a skull twists or bends under loading. If,  
541 instead of landmarks the coordinates of all nodes of the finite element mesh are submitted to  
542 analysis, strains can be computed from the coordinates of the unloaded and loaded meshes.

543 On the other hand the concentrations of stresses or strains in localised regions are useful  
544 predictors of failure and while the overall distribution of strains can be used to infer global  
545 modes of deformation this requires simultaneous interpretation of one contour map for each  
546 principal strain (2 in 2D analyses and 3 in 3D). Thus the approaches can be considered  
547 complementary. GM analyses inform with regard to how loading deforms an object, in terms

548 of changes in size and shape. On the other hand, stresses and strains inform with regard to the  
549 likelihood of failure in particular anatomical regions and how distributions of high and low  
550 strains may eventually relate to (re)modelling fields. Each can be used to infer the other, thus  
551 GM analyses that use the coordinates of the nodes of an FE mesh result in visualisations of  
552 deformations of that mesh and strains can be computed and displayed in these meshes, while  
553 strains can be used to infer global degrees and modes of deformation. It should be noted that  
554 the metric of the GM analysis, the Procrustes size and shape distance relates to changes in  
555 size and shape, not the risk of failure. It differs from metrics derived from strains. These  
556 describe different aspects of deformation that are complementary, but not coincident, in  
557 interpreting FEA results.

558

559 Beyond sensitivity analyses, GM methods have been extended to the task of comparing  
560 deformations among different specimens modelled and loaded in equivalent ways (Milne and  
561 O'Higgins, 2012, O'Higgins and Milne, 2013). In this case the analysis focuses on differences  
562 in vectors of deformation rather than the differences between unloaded forms. This is  
563 achieved by computing deformations as differences between registered loaded and unloaded  
564 forms. They can be visualised by adding these vectors to a convenient unloaded form such as  
565 the mean of all unloaded specimens. Beyond comparisons of deformation, it is also possible  
566 to use GM approaches to assess the association between deformation under loading and other  
567 interesting factors such as skeletal form or ecological variables through regression of PLS  
568 analyses. This has not yet been much exploited in the literature but is likely to increasingly be  
569 taken up as a useful approach to the interpretation of the biological significance of differences  
570 in modes and magnitudes of variation. Differences among models in size, applied forces and  
571 material properties can be taken into account by 'correcting' the magnitudes of deformations  
572 according to the known scaling relationships described above.

573

574 The application of GM methods in conjunction with FEA is as yet in its infancy. There are  
575 clear roles for GM methods in reconstruction, the production of models with modified  
576 geometry to explore how form and function interact and in comparing the results of FEAs  
577 among models and load cases. Each of these approaches has potential benefits and pitfalls  
578 and, in time, with increasing numbers of studies applying these methods we will better  
579 understand where they are applicable and where not. At present these combined GM/FEA  
580 approaches are still fairly novel and some years of methodological development can be  
581 anticipated.

582

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589

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591

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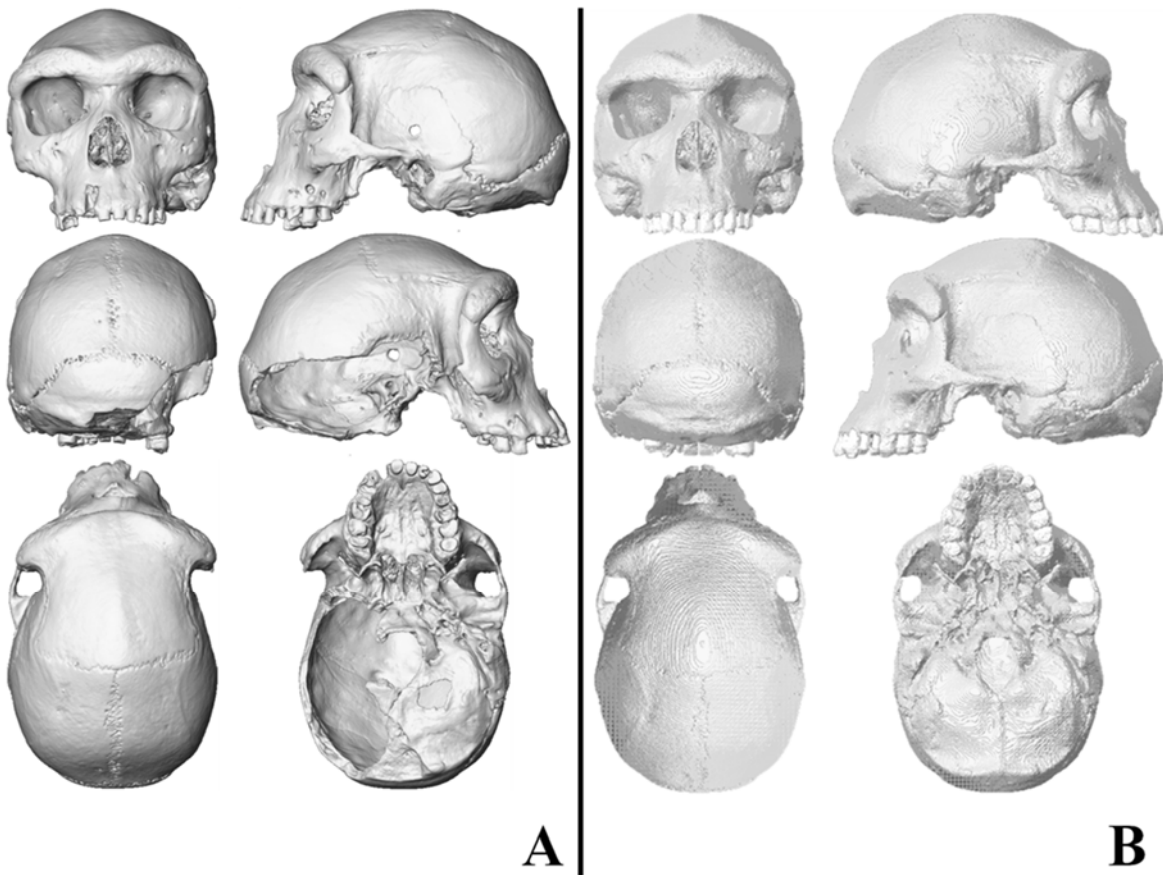
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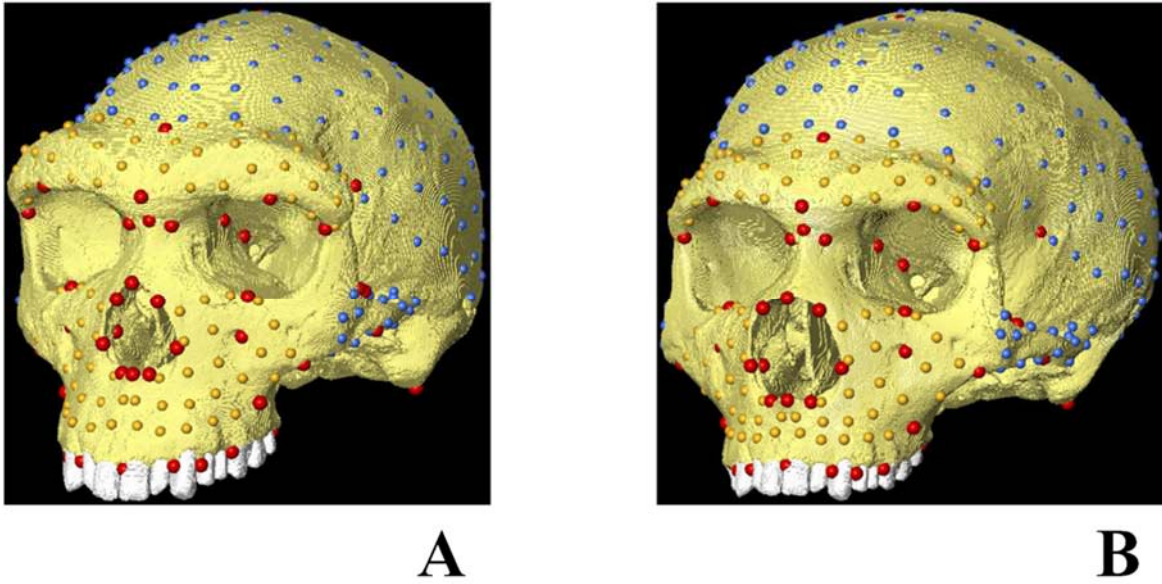
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863 Figure 1: Cranium of Kabwe 1 (A) before and (B) after reconstruction.

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868 Figure 2: A reconstructed Kabwe 1, *Homo heidelbergensis* cranium model (A) and a  
869 hypothetical *Homo neanderthalensis* (B). The hypothetical Neanderthal was created via  
870 surface warping model A into a mean Neanderthal landmark data set (B) using thin plate  
871 splines based on classical and sliding semi-landmarks. Conventional landmarks (red spheres);  
872 sliding semi-landmarks on the maxilla and brow-ridge (yellow spheres); sliding semi-  
873 landmarks of the vault and zygoma (light blue spheres).

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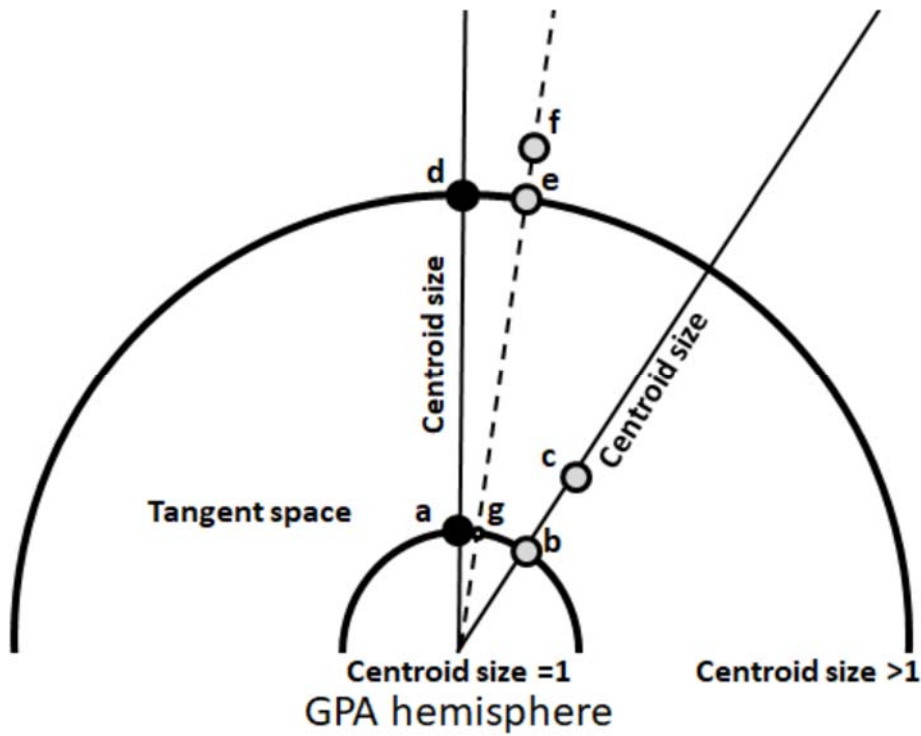


Figure 3: A schematic illustrating the hemisphere of GPA aligned coordinates (Slice 2001) for triangles, showing the tangent space, the vectors of centroid size, and the size and shape space resulting from rescaling of GPA registered coordinates to centroid size  $>1$ . The black points, a and b, represent the same unloaded forms with different centroid sizes. The grey points c and f represent the loaded forms and the grey points b and e represent their projections onto the GPA hemispheres with centroid sizes  $=1$  and  $>1$ . G is the projection of f and e onto the GPA hemisphere with centroid size  $=1$ . See text for explanation.

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902 Figure 4: PCA of large scale deformations of a sensitivity study assessing the impact of  
903 simplifications of material properties in a modern human cranium. Model 1 is not visible  
904 because it is in the same location in the plot as model 2. Deformations are magnified by a  
905 factor of 500 to facilitate visualisation.

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