



## Morphometry of upper cheek teeth of cave bears (Carnivora, Ursidae)

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Univariate and multivariate statistics were applied to analyse the morphometrical variability of 4920 upper cheek teeth (P4, M1 and M2) of cave bears from 123 geographical sites (180 samples) of different Pliocene – Pleistocene ages. The analysed specimens included those belonging to the big cave bears *Ursus kudarensis*, *U. deningeri*, *U. spelaeus* (three subspecies) and *U. kanivetz* (including *U. ingressus*), as well as the small cave bear *U. rossicus*. The information-theoretical parameters (Shannon entropy and orderliness (Von Foerster, 1960: On self-organizing systems and their environments. *In* Self-Organizing Systems, 31–50. Pergamon Press, London) were used to estimate tooth diversity in different teeth, different taxa and in selected local chrono-populations. Multivariate allometry coefficients (Klingenberg, 1996: Multivariate allometry. *In* Advances in Morphometrics, 23–49. Plenum Press, New York) were used to describe the relationships of different ‘parts’ of a tooth and to compare allometric patterns amongst species or selected local samples. A multivariate analysis showed a significant overlap of the size/shape parameter ranges in deningeroid and spelaeoid bears within morphological spaces. Within the cave bear lineage, the Deninger’s bear has the greatest morphological diversity index (entropy) of all the teeth overall, and the lowest diversity is observed in the final taxon of this lineage – *U. kanivetz* (= *ingressus*). The P4 and M2 diversity showed multidirectional correlations with elevation above sea level amongst several ‘local’ populations of Late Pleistocene cave bears. The morphological disparities between the studied taxa are in close agreement with the distances in the available schemes of genetic differentiation based on ancient mitochondrial DNA. The split of *U. kudarensis* and *U. deningeri* has a good bootstrap support, which corresponds to the hypothesis about their parallel evolution. The small cave bear *U. rossicus* is placed between *U. arctos* and *U. deningeri*. The phylogenetic signal is more pronounced in the variability of teeth in comparison with other skeletal remains of cave bears (cranium, mandible, or metapodial bones).

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Cave bears are amongst the most famous representatives of the European Ice Age fauna. Their bone remains were originally reported known from many Middle and Late Pleistocene cave localities from Great Britain and Spain in the west to the Urals in the east (Kurtén 1968, 1976; Rabeder *et al.* 2000). Later, research found that the range of cave bear distribution extended far beyond the limits of Europe, and their remains were found in Siberia (as far as Transbaikalia and the Kolyma River in the east), in western (Caucasus, Israel) and central (Kazakhstan, Kirghizia) Asia and on the Korean Peninsula (Baryshnikov 2007; Knapp *et al.* 2009; Sher *et al.* 2011).

Recent studies show a significant genetic diversity of cave bears (Valdiosera *et al.* 2006; Rabeder *et al.* 2008, 2010, 2011; Knapp *et al.* 2009; Dabney *et al.* 2013; Stiller *et al.* 2014). Analyses of ancient mtDNA revealed several evolutionary lineages, which are frequently regarded as separate species: *Ursus spelaeus* Rosenmüller, 1794 (Late Pleistocene, western Europe and west Siberia), including subspecies *U. s. eremus* Rabeder, Hofreiter, Nagel *et al.* Withalm, 2004 (the Alps and Altai Mountains) and *U. s. ladinicus* Rabeder *et al.*, 2004 (highlands in Alps), *U. deningeri* von Reichenau, 1904 (Middle Pleistocene, Europe and central Asia), including subspecies *U. d. batyrovi* Baryshnikov, 2007 (Kirghizia), *U. kanivetz* Vereshchagin, 1973 (= *U. ingressus* Rabeder *et al.*, 2004) (Late Pleistocene, central and eastern Europe and the Urals), and *U. kudarensis* Baryshnikov,

1985 including subspecies *U. k. praekudarensis* (Baryshnikov 1998) (Middle and Late Pleistocene, Caucasus and, probably, eastern Siberia).

Genetic data revealed an earlier splitting of *U. kudarensis*, whereas *U. spelaeus* and *U. kanivetz* (= *ingressus*) separated later from *U. deningeri* (Valdiosera *et al.* 2006; Baca *et al.* 2012, 2016; Fortes *et al.* 2016). According to Dabney *et al.* (2013), *U. deningeri* forms a sister lineage to *U. spelaeus* and *U. kanivetz* (= *ingressus*). Early Pleistocene *Ursus etruscus* G. Cuvier, 1823, is considered the ancestor of cave bears, which had a Palaearctic distribution (Kurtén 1968).

Cave bears from the Urals (Russia) are grouped, according to the genetic data, with cave bears from eastern Europe belonging to the haplogroup ‘*ingressus*’ (Baca *et al.* 2012, 2016; Stiller *et al.* 2014); however, a craniometrical difference was detected between these two populations (Baryshnikov & Puzachenko 2011). Therefore, we analysed two separate geographical samples: *U. k. kanivetz* (Urals) and *U. k. ingressus* (eastern Europe up to the Volga River).

Another species, *U. rossicus* Borissiak, 1930 (including subspecies *U. r. uralensis* Vereshchagin, 1973), represents the smallest cave bear in the Middle and Late Pleistocene of eastern Europe, the Urals and western Siberia (Vereshchagin & Baryshnikov 2000; Spassov *et al.* 2017). Baryshnikov (2007) integrated it with *U. savini* Andrew, 1922, from the Middle Pleistocene of England

(Forest Bed), whereas Spassov et al. (2017) suggested recently distinguishing between *U. savini* (including *U. rossicus*) and *U. uralensis*. According to mitochondrial evidence, *U. rossicus* occupies the basal position in the lineage of ‘ingressus’ (Stiller et al. 2014), but is morphologically peculiar (Baryshnikov & Puzachenko 2011, 2017).

Museum collections include many thousands of cave bear teeth recovered from cave localities, these teeth being repeatedly examined by palaeontologists (Baryshnikov 1998, 2006; Rabeder 1999; Rabeder et al. 2008, 2010, 2011; Wagner & Čermák 2012). We performed a new analysis of morphometrical diversity of cave bear teeth, with the use of methods of multivariate statistics. Such studies can help to define the morphological space of the groups, which may consequently be compared with those of other mammal taxa.

The present contribution continues our previous study of cave bears; several works have been already published on skull variability (Baryshnikov & Puzachenko 2011), metapodial bones (Baryshnikov & Puzachenko 2017), and mandibles (Baryshnikov et al. 2018). As a large amount of material has been obtained, we divided our new study into two contributions: one considering the upper cheek teeth (this paper) and another – lower cheek teeth (in preparation).

As a starting point, we will consider several views on the causes of evolution of dentition morphology of cave bears and formulate several hypotheses of morphometric variation, which will be tested by the results of the analyses performed.

Through the Pleistocene, the cheek teeth of cave bears demonstrate progressive modification of the occlusal surface, and the rate of such changes increases toward the end of this epoch (Rabeder & Tsoukala 1990; Rabeder 1999). It has been also found that sites of the same age are geographically grouped with regards to cave bear dental measurements. This phenomenon may be explained by regional peculiarities in the bear diet (Taboda et al. 2001; Baryshnikov et al. 2003, 2004; Bocherens et al. 2014; Robu et al. 2018), as well as by other environmental factors (elevation of habitat above sea level, physiography, and climate evolution; Jambrešić & Paunović 2002; Athen et al. 2005; de Carlis et al. 2005; Santi & Rossi 2005; Toškan 2006; Rabeder et al. 2008, 2010, 2011; Toškan & Bona 2012; Krajcarz et al. 2016; Robu 2016), and/or by philopatry that suggests limited movement of bears during their lifetime that imposes constraints on the gene flow (Ábelová 2006; Fortes et al. 2016).

Most studies of cave bear tooth morphology and morphometry, as well as those of their skull and postcranial elements, are based on geographically restricted material. Our previous studies (Baryshnikov & Puzachenko 2011, 2017) have shown that the inclusion of data recovered from widely spaced sites and belonging to various genetic groups lead to significant changes in views on the morphological variability in cave bears.

Typically, the morphological ‘gaps’ are found between species or subspecies of cave bears when the compared morphometric data are obtained from a small number of localities. In cases in which the considered materials are recovered from many sites, the variability becomes practically continuous. The results of an analysis depend critically on the geographical position of the sources (local level – several nearby caves, regional level, or the entire range of the species) and on their relative age (layers of the same or different age). Numerous investigations have demonstrated that cave bear morphological variability is highly complex regardless of the spatial and temporal scales.

The main aim of our review is to present the morphometry of upper premolar (P4) and molar (M1, M2) teeth (Fig. 1) sampled from numerous Eurasian sites of different geological ages and geographical positions in order to elucidate their variability beginning from the Pliocene *U. minimus* Devèze de Chabriol et Bouillet, 1827, and the Early Pleistocene *U. etruscus*, to the youngest cave bears from the Late Pleistocene.

We also study the variability of the cheek teeth in the brown bear *U. arctos* Linnaeus, 1758, which evolved in parallel to cave bears in the Pleistocene but now represents an undoubted evolutionary success unlike the extinct cave bears. In this work, we excluded from the analysis the most controversial taxa and problematic samples, such as *U. savini*, *U. suessenbornensis* Soergel, 1926 (Rabeder et al. 2010; Spassov et al. 2017), and several ‘early’ cave and brown bears from European localities dated to the early Middle Pleistocene. Those are scheduled to be considered separately later, after a review of the lower cheek teeth.

We propose to produce morphometric data in forms making it possible to check the presence of phylogenetic signal in the variability of the tooth size and shape; to provide a basis for a morphometric classification; to study temporal patterns in tooth size and shapes; to study the multivariate allometry pattern; and to estimate morphological diversity parameters in the studied ursids.

In addition, we wanted to test some basic hypotheses about morphological diversity. The first hypothesis assumes no difference between morphological (=morphometrical, in this case) diversity amongst upper cheek teeth. The alternative is that the maximum diversity

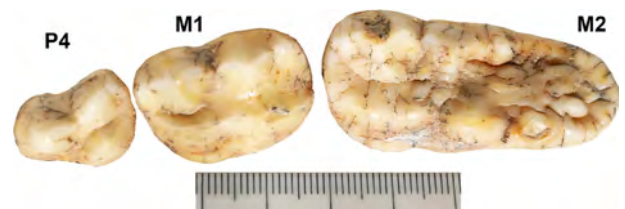


Fig. 1. Left upper teeth row P4–M2 of the cave bear *Ursus kudarensis praekudarensis* (ZIN 31896, Kudaro 1 cave, layer 5c, Middle Pleistocene); occlusal view.

should be found in the second molar M2 or premolar P4, and the lowest diversity in the first molar M1, according to the inhibitory cascade model (Kavanagh *et al.* 2007). This assumption is based on the conjecture that the first molar's variation is probably limited by both the premolar and second molar. The next hypothesis assumes that there is no difference between the Middle Pleistocene *U. deningeri* and the Late Pleistocene cave bears (*U. spelaeus* s. str. or *U. kanivetz* (= *ingressus*)) in terms of diversity parameters. An alternative hypothesis is based on the assumption of a decrease in morphological diversity as consequences of consumption of mostly food.

## Material and methods

### Material

The study was based on 180 teeth samples of different Pliocene – Pleistocene ages that were recovered from 123 geographical localities (some of them are multilayered) in Europe, the Caucasus, Siberia, Central Asia and northern Africa (Fig. 2, Table S1). 4920 fossil upper cheek teeth (P4 – 1463, M1 – 1715, M2 – 1742; Tables 1, S1) belonging to *U. minimus*, *U. etruscus*, *U. deningeri*, *U. kudarensis*, *U. rossicus*, *U. savini*, *U. spelaeus*, *U. kanivetz* (= *ingressus*) and fossil *U. arctos* were examined. In addition, 525 teeth (P4 – 178, M1 – 170, M2 – 177) of recent brown bear subspecies (*U. a. arctos* Linnaeus, 1758, *U. a. yessoensis* Lydekker, 1897, *U. a. pruinosus* Blyth, 1854, *U. a. meridionalis* Mitterdorff, 1851, *U. a. piscator* (Pucheran, 1855) and *U. a. gyas* Merriam, 1902) were examined.

The scheme of measurements of the upper cheek teeth (Baryshnikov 2006) and indexes are shown in Fig. 3. All the measurements were performed using callipers to the nearest 0.01 mm.

One of the authors (G. F. Baryshnikov) examined collections from 24 depositories. The most important samples and localities of *U. deningeri* are: (i) Mosbach (NHMM, NSMW; 138 teeth; Mosbach 2: ~0.62–0.48 Ma BP (Maul *et al.* 2000), Germany), (ii) Einhornhöhle (Unicorn Cave) (NLM; 162 teeth; ~0.85–0.50 Ma BP (Athen 2007), Germany), (iii) Koněprusy (NMP; 176 teeth; ~0.73 Ma BP (Wagner 2001), Czech Republic), (iv) Westbury-Sub-Mendip (NHM; 119 teeth; ~0.42 Ma BP, MIS 11 (Bishop 1982), UK). The important samples of *U. k. praekudarensis* were collected from layer 5 of Kudaro 1 Cave (ZIN; 147 teeth; ~0.36–0.24 Ma BP (Liubin 1998), Georgia) and of *U. k. kudarensis* – from layers 3–4 of Kudaro 3 Cave (ZIN; 85 teeth; ~0.09–0.04 Ma BP (Baryshnikov 2011) and Malaya Vorontsovskaya Cave (ZIN; 75 teeth; ~0.05–0.03 Ma BP (Golovanova & Doronichev 2005), Russia). Amongst *U. spelaeus* the following samples should be noted: (i) Baumannshöhle (Rübeland) (MNHUB; 137 teeth, ~0.046–0.039 Ma BP (Rosendahl *et al.* 2005), Germany), (ii) Zoolithen Cave (IPE; 197 teeth; ~0.06–0.03 Ma BP (Hilpert *et al.* 2005), Germany), (iii) Goyet Cave (IRNHB; 115 teeth; ~0.041–0.028 Ma BP (Naito *et al.* 2016 and others), Belgium), (iv) Ramesch-Knochenhöhle (IPV; 191 teeth; ~0.04 Ma BP (Fiebig & Pacher 2006), Austria), (v) Schwabenreith (IPV; 167 teeth; ~0.11–0.039 Ma BP (Döppes *et al.* 2016), Austria), and (vi) Conturines cave (IPV; 228 teeth; ~0.11–0.048 Ma BP (Döppes & Rosendahl 2009), Italy). The set

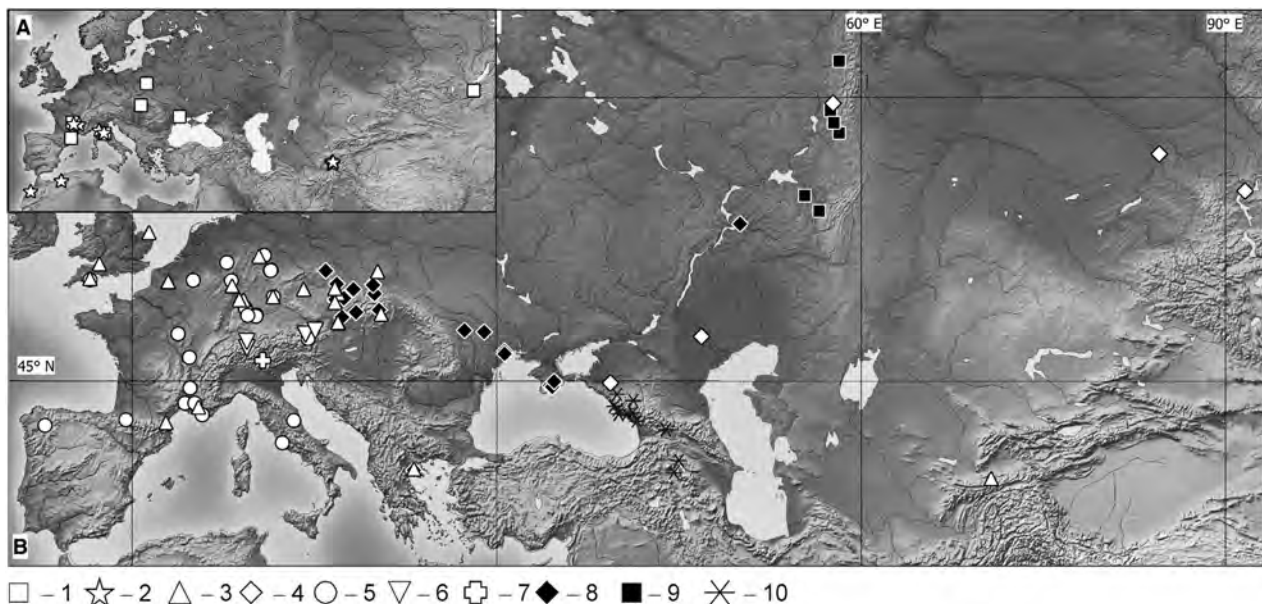


Fig. 2. Distribution of examined localities of the fossil bear except *Ursus arctos*: 1 = *U. minimus*; 2 = *U. etruscus*; 3 = *U. deningeri*; 4 = *U. rossicus*; 5 = *U. s. spelaeus*; 6 = *U. s. eremus*; 7 = *U. s. ladinicus*; 8 = *U. kanivetz ingressus*; 9 = *U. k. kanivetz*; 10 = *U. kudarensis*.

Table 1. The samples of upper cheek teeth used in this study.

Taxon	Number samples	of	Number of teeth			Total
			P4	M1	M2	
<i>U. minimus</i>	7		8	13	14	35
<i>U. etruscus</i>	9		18	24	23	65
<i>U. deningeri</i>	24		272	290	302	864
<i>U. kudarensis</i>						
<i>U. k. praekudarensis</i>	12		118	118	82	318
<i>U. k. kudarensis</i>	20		81	63	92	236
<i>U. savini</i>	1		5	3	3	11
<i>U. spelaeus</i>						
<i>U. s. spelaeus</i>	27		275	300	355	930
<i>U. s. eremus</i>	4		134	156	140	430
<i>U. s. ladinicus</i>	1		100	74	54	228
<i>U. kanivetz</i>						
<i>U. k. ingressus</i>	26		238	390	364	992
<i>U. k. kanivetz</i>	8		97	97	101	295
<i>U. rossicus</i>	5		23	30	34	87
<i>U. arctos</i> (fossil)	36		94	157	178	429
<i>U. a. arctos</i> (recent)	1		51	51	51	153
<i>U. a. piscator</i> (recent)	1		30	30	30	90
<i>U. a. meridionalis</i> (recent)	1		20	21	20	61
<i>U. a. pruinus</i> (recent)	1		23	21	23	67
<i>U. a. yesoensis</i> (recent)	1		54	46	53	153
<i>U. a. gyas</i> (recent)	1			1		1
Total	186		1641	1885	1919	5445

of important localities of *U. kanivetz* (= *ingressus*) includes (i) Il'inka (NMNH; 294 teeth; approximately dated to MIS 4–MIS 3 time, Ukraine), (ii) Odessa-Nerubaj caves (PIN, FNH; 159 teeth; ~0.07 Ma BP (Nagel *et al.* 2005; Valde-Nowak *et al.* 2016), Ukraine), (iii) Gamssulzenhöhle (IPV; 128 teeth; ~0.05–0.03 Ma BP (Kavcik-Graumann *et al.* 2016), Austria), (iv) Secrets cave (ZIN; 181 teeth; ~0.043–0.031 Ma BP (Kosintsev *et al.* 2016), Russia), and (v) Medvezh'ya Cave (ZIN; 62 teeth; ~0.05–0.015 Ma BP (Kosintsev *et al.* 2016), Russia). The material (80 teeth) of *U. rossicus* came from the Kizel Cave (Viasher cave) (ZIN; ~0.05–0.02 Ma BP 2 (Pacher *et al.* 2009; Kosintsev *et al.* 2016), Russia). The most important localities of *U. etruscus* are (i) Saint-Vallier (CCML; 24 teeth; ~2.4 Ma BP (Guérin *et al.* 2004), France), (ii) Olivola (IGF, MNHN; 17 teeth, ~1.9 Ma BP (Palombo *et al.* 2008), Italy), and (iii) Val d'Arno (IGF; 13 teeth; ~2.5 Ma BP (Napoleone *et al.* 2003), Italy). Finally, the largest sample of *U. minimus* material (13 teeth) for this study comes from the Węże 1 site (ISEA; ~4.8–3.4 Ma BP (Mein 1989), Poland).

Institutional abbreviations are: CCML, Collections of Confluences Museum, Lyon, France; FNH, Finnish Museum of Natural History, Helsinki, Finland; GIUC, Geological Institute, University of de Coruña, Spain; HNHM, Hungarian Natural History, Budapest, Hungary; IGF, Museum of Natural History, University of

Florence, Italy; IPE, Institute of Paleontology, Erlangen, Germany; IPV, Institute of Paleontology, Vienna, Austria; IRNHB, Royal Institute of Natural History, Brussels, Belgian; ISEA, Institute of Systematics and Evolution of Animals, Kraków, Poland; MMB, Moravské Museum, Brno, Czech Republic; NMP, National Museum, Prague, Czech Republic; MNHUB, Museum of Natural History, Humboldt University, Berlin, Germany; MNHN, Museum of Nature History, Paris, France; NHM, Natural History Museum, London, UK; NHMM, Natural History Museum, Mainz, Germany; NLM, Niedersächsisches Landesmuseum, Hannover, Germany; NMNH, National Museum of Natural History of National Academy of Sciences Kiev, Ukraine; NSMW, Natural History Collection, Museum Wiesbaden, Germany; PIN, Borissiak Paleontological Institute of the Russian Academy of Sciences, Moscow, Russia; SMNH, State Museum of Natural History, Stuttgart, Germany; SNM, Slovak National Museum, Bratislava, Slovakia; ZIN, Zoological Institute of the Russian Academy of Sciences, Saint Petersburg, Russia.

### Missing data

To estimate missing measurements (due to damaged skulls), we used the expectation-maximization (EM) algorithm (Dempster *et al.* 1977). In all cases, the 'at random' hypothesis was accepted for completely missing measures (Pigott 2001). EM estimates the means, covariance matrix and correlation of measures with missing values, using an iterative process. The Grubbs two-sided test (Stefansky 1972) was used to reveal outliers in variables with filled missing values. Statistical differences between measurements (average, variance, type of distribution) were tested by comparing the data set, including missing values filled in by the EM method, to the initial data set. No statistical differences were detected between the two data sets. We used estimated values for multivariate analysis only.

### Sexual size dimorphism

As sexual size dimorphism (SSD) can be a potentially important factor with respect to the size variation in cheek teeth (Kurtén 1955; de Torres *et al.* 2002; Baryshnikov *et al.* 2003, 2004; Baryshnikov 2006), we developed a general test for sex determination based on cheek teeth dimensions. The test was applied to the examples of partially a priori sexed samples of recent brown bears, which belong to *U. a. arctos*, *U. a. piscator*, *U. a. pruinus*, *U. a. meridionalis* and *U. a. yesoensis* (Data S1). We used natural logarithms of all the tooth measures and principal components analysis (PCA) for the description of the general size variability of a tooth. Then, PC1 was used as a variable for the partition of a sample into two clusters – 'large' and 'small' teeth (*K*-means and hierarchical UPGMA method used for comparison). The

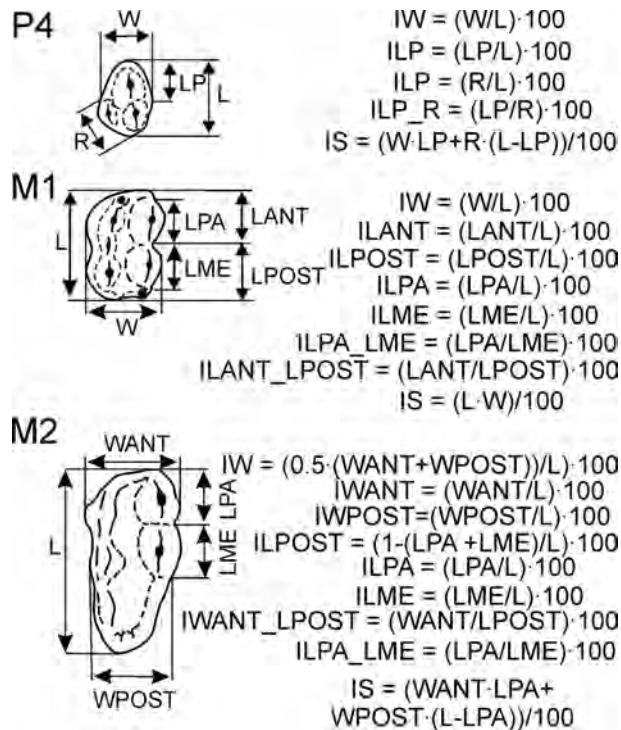


Fig. 3. Measurements of the upper premolar (P4) and molars (M1, M2) (Baryshnikov 2010) and indexes used in this study. L = greatest length; W = greatest width; LP = length of P4 paracone; LPA = length of paracone in M1 and M2; LME = length of metacone; R = least distance between frontal ridge of protocone and posterior side of crown of P4; LANT = length of anterior part of M1; LPOST = length of posterior part of M1; WANT = greatest width of M2; WPOST = talon width through hypocone of M2; IS = index of masticatory surface area of P4–M2; IW = roundedness index of P4–M2; ILP, ILPA = paracone indexes; ILME = metacone index; ILP\_R = protocone–paracone index of P4; ILANT\_LPOST = anterior–posterior index of M1; ILPA\_LME = paracone–metacone index of M1 and M2.

teeth, which were classified equally by all the clustering techniques ('large' teeth belonged to males and 'small' ones to females), were grouped into 'learning samples' for further discriminant analysis. Lastly, we compared a priori partitions of males and females based on museum labels with new ones determined by discriminant analysis. The average mismatch between a priori sex and estimated sex was 25–32%. The maximum incompatibility (about 50%) was observed in the small-sized subspecies *U. a. meridionalis*. Generally, the result of the sex determination by cluster analysis leads to an overestimation of SSD contribution in most studied cases (Data S1). In recent brown bear subspecies, the SSD of the cheek teeth is much less pronounced than the dimorphism of the skull (Baryshnikov & Puzachenko 2011) or metapodial bones (Baryshnikov & Puzachenko 2017) and the contribution of SSD to size variability is relatively weak.

Based on these data we conjectured that formal methods of sex determination of recent and, with a high probability, of fossil cheek teeth are inapplicable in the

case of brown and cave bears, because they can lead to a significant misrepresentation of the final results. Therefore, the morphometric analysis in this work was carried out without dividing the sample into males and females.

### Morphological space model

The general approach to morphometric study that we used in this analysis has been described in detail in many of our previous contributions (Puzachenko 2001; Kupriyanova *et al.* 2003; Abramov *et al.* 2009; Baryshnikov & Puzachenko 2011, 2017; Puzachenko *et al.* 2017; for more details see Data S2). We used the nonmetric multidimensional scaling (NMDS) technique (Davison & Jones 1983) to construct two types of multivariate models (morphological space or 'morphospaces') based on matrixes of Euclidean distances and Kendall's tau-b (corrected for ties) associations (Kendall 1975) amongst all pairs of teeth. The Euclidean metric produces a common Euclidean space with an orthogonal coordinate system. The metric based on Kendall's coefficients causes a curvilinear surface, which, as result of NMDS, can be projected onto the Euclidean space as a segment (one dimension), a circle-like figure (two dimensions) or a multidimensional sphere (three and more dimensions). As a result, we used a variant of the morphospace that reproduces the variations in cheek teeth size (SZM model), and another one that reproduces the variations in cheek teeth proportions (shape) (SHM model) (Puzachenko 2016). The dimensionality (*d*) of morphospace (=number of NMDS model axes) is estimated using Kruskal's stress (Kruskal 1964; Kupriyanova *et al.* 2003; Abramov *et al.* 2009; Baryshnikov & Puzachenko 2011, 2012, 2017; Abramov & Puzachenko 2012; Puzachenko *et al.* 2017). The coordinates of a NMDS model based on the Euclidean distance matrix will be denoted in the text as E1, E2... and the coordinates based on Kendall's measure of association matrix will be denoted as K1, K2... Coordinates of morphological spaces are used as generalized variables containing information on the size and shape variability of cheek teeth.

Morphospace coordinates of taxa centroids have been used as variables for hierarchical cluster analysis where the neighbour-joining (NJ) clustering method was used (Saitou & Nei 1987).

### Morphological diversity

We will consider morphological or, in our case, morphometric diversity as a characteristic of any sample, each element of which (in the particular case it is a tooth) is associated with a set of morphometric variables – the measurements. The quantitative variables of morphological diversity, in turn, are parameters of models of morphological spaces. The properties of these models, including the independence of coordinates, make it

possible to use the well-known Shannon's information entropy (Shannon 1949) or any other form of entropy and its derivative, redundancy, also proposed by Shannon (Shannon 1948). The use of models of morphological spaces (see also Data S3) allows us to compare the entropy or derived parameters of samples that include different elements with different sets of measurements, i.e. such as different cheek teeth.

Entropy ( $H$ , bit per element of the sample) of the SZM (or SHM) morphospace has  $d$  coordinates and  $N$  elements calculated as,  $H = -\sum_{j=1}^d \sum_{i=1}^k p_i \log_2 p_i$  where  $p_i = n_i/N$  ( $\sum p_i = 1$ ), and  $k = 1 + \log_2 N$  (Sturges 1926) – rounded number of class intervals (gradations) for the NMDS axes. In this study, we restricted the gradations of NMDS axis partitioning to six intervals;  $1 + \log_2 34 \approx 6$ , where 34 is the minimum sample size of all those for which the calculations were made.

The next derived parameter of diversity is redundancy (Shannon 1948; Pielou 1966), calculated as  $R = 1 - H/(d \log_2 k)$ . The  $R$ -value ranges from 0 (limitations are absent, nondeterministic, stochastic chaotic system) to 1 (extremely strong limitation, full deterministic system). Von Foerster (1960) suggested using the  $R$ -value as a measure of the internal orderliness of complex systems in the processes of their self-organization. In a general case, entropy is linearly dependent on  $\log_{10} N$ . Therefore, in order to compare correctly samples with different number of elements, it is necessary to calibrate the values of entropy or other derived parameters. The calibration of  $H$  (or  $R$ ) is in accordance with the following transformation:  $H_{\text{cal}} = (H - (a + b \log_{10} N)) + (a + b \log_{10} N_{\text{const}})$ . We fix  $N_{\text{const}} = 50$  because the entropy is increasing by  $\sim 3.5\%$  only between  $N = 40$  and  $N = 100$  in case of random normal distribution (Puzachenko 2013; Data S3).

### Multivariate allometry

Allometric relationships act as a mechanism that narrows the potential variability of cheek teeth, thereby influencing morphological diversity. According to Cock (1966) and Klingenberg (1996), there are three variously interrelated concepts of allometry: 'static allometry' reflects variation amongst individuals within a homogeneous age group at the population level; 'ontogenetic, or growth, allometry' deals with variations amongst ontogenetic stages on the species level; 'evolutionary allometry' reflects covariation of characters amongst individuals from different lineages that have a common ancestor (Gould 1966; Klingenberg & Zimmermann 1992). When dealing with palaeontological material in studies of static allometry, quite often it is not clear whether the samples under study belong to a 'single population', even if the remains were excavated from one site and even from the same layers. In addition, the material can relate to a considerable time interval, during which the characteristics of organisms could change in a

certain direction. Therefore, the study of allometry using palaeontological material is associated with difficulties in interpreting the results and requires additional hypotheses.

The study of ancient mtDNA and strontium isotope ratios (Ábelová 2006; Fortes et al. 2016) suggests extreme fidelity of cave bears to their birth site, at least in females, and limited movement of bears during their lifetime. In this study, we also consider the allometric relationship between the characteristics (measurements) of the cheek teeth of adult animals only. This allows us to consider the local samples as samples from geographical 'chrono-populations' and our interest was focused on the constraints imposed on morphological diversity associated with a pattern of evolutionary allometry.

A PCA of the covariance matrix of log-transformed measurements was used for calculation of the multivariate allometric coefficient (MAC) according to Jolicoeur (1963), Klingenberg & Froese (1991) and Klingenberg (1996). According to Jolicoeur (1963), the coefficient (loading or eigenvalue) of a given measurement on a first principal component (PC1) divided by  $1/\sqrt{m}$  (where  $m$  is the number of measurements) is MAC. The 95% confidence intervals for MACs were estimated using the bootstrap method (100 iterations for each sample).

In the geometric model, MAC corresponds to the angle between PC1, which correlates with the 'general size' of a tooth, and separate measurements of a tooth. MAC values  $>1.0$  indicate positive allometry,  $\text{MAC} \approx 1.0$  suggests isometry, and  $\text{MAC} < 1.0$  is indicative of negative allometry.  $\text{MAC} \approx 0$  indicates a case when the variation of a given measurement is completely independent from the 'general size' of the tooth (allometry is absent). The composition of positive and negative allometry results in differences in the shapes of a particular tooth between taxa or amongst several chrono-populations.

If a model includes all studied taxa of bears (general model, GPC), then the first component (GPC1) corresponds to a 'baseline' in relation to all other particular PC1s of taxon-specific PCA models. The angle in degrees between the GPC1 and a particular PC1 in Euclidean coordinate space ( $\text{GPC1} \times \text{PC1}$ ) is calculated as  $\arctan b \cdot (180^\circ/\pi)$ , where  $b = |b_i - b_{\text{bas}}|$ , and  $b_i$  is the coefficient of linear regression in the equation  $\text{PC1}_i = a + b_i \text{GPC1}$ . If  $b_{\text{bas}} = 1$ , the angle between GPC1 and PC1 is  $45^\circ$ . In the same way, it is possible to calculate the angles between the first components of any particular specific models. When the pair of PC1s is compared, the sign of ' $b$ ' does not matter, but if several PC1s are pairwise compared, the sign is significant; it indicates which direction (clockwise or counterclockwise) they deviate relative to each other.

Thus, in this study, within the framework of the multivariate allometry analysis, we obtained two new sets of variables describing the morphometric variability of teeth – the MACs and the angles ( $\gamma$ ) between the size

allometry patterns in different taxa or chrono-populations.

The statistical analysis was carried out with STATISTICA v. 8.0 (StatSoft, Tulsa, OK, USA), PAST v. 3.12 (Hammer *et al.* 2001) and NCSS 12 Statistical Software (ncss.com/software/ncss).

## Results

### *Morphological spaces and their interpretations*

**P4.** – The dimensionalities of the SZM and SHM morphospaces of P4 were 2 and 3, respectively (Table 2). The linear multiple regression models of P4 measures with morphospace dimensions have high coefficients of determination ( $r^2$ ) showing that all meaningful information about P4 variability is contained in variation of the morphospace dimensions. The coordinates of the two morphospaces describe 97–98% of the variation in the row measurements.

In the SZM model, the first dimension (E1) describes the ‘general size’ of the tooth because high correlations with all P4 measurements are observed (Fig. 4A). Furthermore, E1 correlates with the index of masticatory surface area (IS;  $r = 0.99$ ), thus P4 surface area in all taxa depends on the ‘general size’ directly (Table 2). The second coordinate of SZM (E2) describes the variation of several indexes – ILP\_R, IR and IW, therefore, it reproduces an allometric pattern of the P4 shape variability. E1 correlates with the first coordinate of the SHM model (K1), which describes some aspects of P4 shape. Coordinate K2 shows low correlation with the roundness index (IW), herewith relatively high correlation coefficients were obtained for several taxa (*U. deningeri*, *U. k. praekudarensis*, *U. s. spelaeus* and

*U. k. kanivetz*) (Data S4). The last coordinate of the SHM morphospace (K3) correlates with ILP (Table 2).

The percentage of variance of E1 that explained by a taxonomical composition of sample (factor “TAXA”, Table 2) is 49.3% if brown bear, *U. minimus* and *U. etruscus* were included and only about 25% if last three species were excluded from the analysis. The amount of variances of K1–K3 coordinates (SHM model) explained by the factor “TAXA” were between 28 and 16.1 percentages.

These results suggest a considerable overlap of taxa ranges in morphological space. According to Fig. 4B, the morphometric variability of P4 is continuous overall, from *U. minimus* through *U. etruscus* to the largest representatives of the cave bear lineage. Nevertheless, some specific features of P4 in different taxa should be discussed in terms of the general background of continuous variability. The centroids of the *U. kudarensis* subspecies are separated from the centroids of the *U. spelaeus* subspecies, but they are close to the *U. deningeri* centroid along the second coordinate, E2. P4 of the Kudaro bear has the lowest protocone–paracone index (ILP\_R: 77–78%, Data S4). In this index (Fig. 3), parameter *R* is determined by the size of the protocone and presence or absence of its anterior additional cusp, as well as by the protocone location, as in the course of ursid evolution this cusp shifted backwards (Baryshnikov 2007). Thus, this evolutionary lineage is characterized by a large P4 with a very pronounced dominance of the protocone complex over the paracone, especially in the final stage of evolution – *U. k. kudarensis*. The protocone–paracone index in Deninger’s bear and brown bear are about 81%, but for all the other taxa it is more than 86% on average, including *U. minimus* (89.1%), *U. etruscus* (85.7%), up to the local species *U. savini* (92.8%) (Data S4).

*U. kanivetz* (= *ingressus*) and *U. s. spelaeus* have the largest P4 with average L about 20 mm. *U. k. kanivetz* has a less developed protocone (ILP\_R: 92.1%) in comparison with other big cave bears. The dimension and shape of P4 in *U. k. ingressus* and *U. s. spelaeus* are very close to each other, but statistically significant differences between these taxa are found in the greatest length of P4, the length of the paracone and in the IS index: 2.9 in *U. s. spelaeus* vs. 3.1 in *U. k. ingressus* (Data S4). The centroid of the next cave bear subspecies, *U. s. eremus*, is placed close to the centroid of *U. k. kanivetz*, according to their similarity in ‘general size’. *U. s. eremus* has a somewhat more developed protocone (protocone–paracone index 74.7%) relative to *U. k. kanivetz* (71.1%).

The centroid of the small *U. s. ladinicus* is placed near the centroids of *U. rossicus* and *U. deningeri* along the E1 coordinate, and so it is separated from the main cave bear cluster. At the same time, the P4 of *U. s. ladinicus* is very similar to this premolar in *U. rossicus*. There are no statistically significant differences between the two taxa,

Table 2. Pearson correlation coefficients of the coordinates of the SZM and SHM morphological spaces (E, K) and measures of P4 and their indexes (variables);  $v$ , ‘TAXA’ = relative variance (%) of dimensions associated with taxonomical composition of samples;  $r^2$  = coefficients of determination of linear multiple regression models:  $\text{var} = A + b \cdot E1 + b1 \cdot E2 + b2 \cdot K1 + b3 \cdot K2 + b4 \cdot K3$ .

Variables	Dimensions of the morphospace					$r^2$
	SZM		SHM			
	E1	E2	K1	K2	K3	
L	0.96	−0.19	−0.27	−0.01	0.45	0.98
LP	0.92	−0.34	−0.43	0.02	0.16	0.98
W	0.93	0.25	0.13	0.25	0.30	0.97
R	0.88	0.39	0.23	−0.14	0.24	0.97
IW	−0.08	0.75	0.72	0.50	−0.27	0.84
ILP	0.13	−0.43	−0.46	0.09	−0.59	0.69
IR	0.02	0.87	0.77	−0.17	−0.29	0.88
ILP_R	0.04	−0.92	−0.86	0.18	−0.08	0.92
IS	0.99	0.08	−0.04	0.04	0.39	0.99
$v$ , ‘TAXA’, full sample	49.3	26.6	28.0	16.6	16.1	
$v$ , ‘TAXA’, cave bears	24.8	25.8	24.2	14.7	5.76	

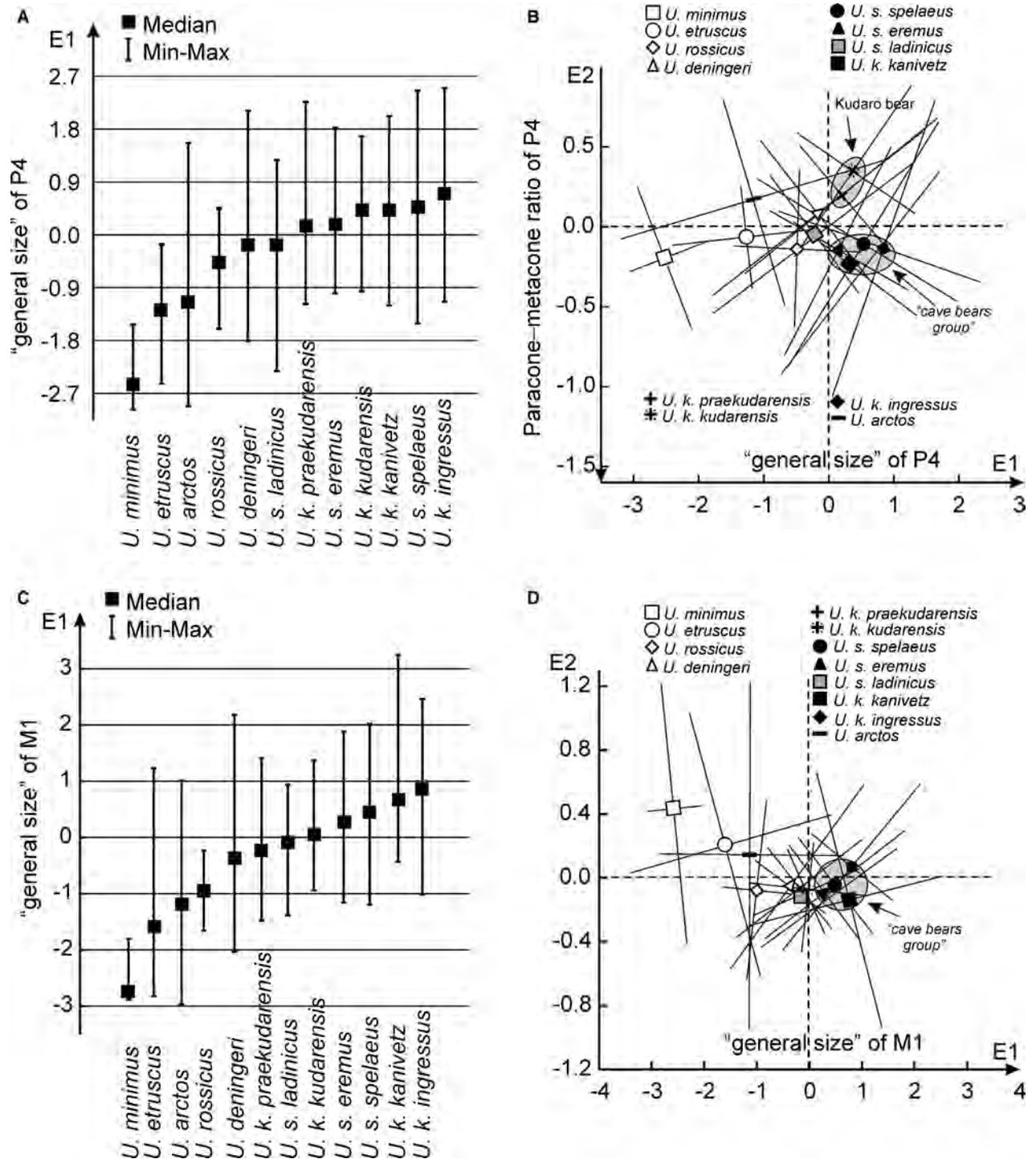


Fig. 4. A, C. Medians and min.-max. of first (E1) coordinate in the bear taxa in SZM morphospaces of P4 (A) and M1 (C). B, D. Centroids and ranges of the bear taxa within SZM morphospaces of P4 (B) and M1 (D). Ranges are equal to sample mean (centroid)  $\pm$  highest value – lowest value  $\times 0.95$ .

except for a minor difference in the paracone index (ILP: 64.9% vs. 66.9%). Minor differences between *U. s. ladinicus* and *U. deningeri* on the ILP and ILP\_R indexes (Data S4) are also found in the ILP and ILP\_R indexes (Data S4).

**M1.** – The dimensionality of both the SZM and SHM morphospaces of M1 is 2. The first coordinates (E1, K1) account for 78–97% of measurement variability (Data S4). E1 describes the 'general size' of M1 (Fig. 4C) and it closely correlates with all measurements of M1 ( $r$  varies

from 0.80 to 0.95). In addition, E1 is strongly correlated with the index of masticatory surface area ( $r = 0.98$ ). The second dimension (E2) is not in linear correlation with any of the M1 measurements. More detailed study has shown significant positive correlations between E2 and the L, LA and W in *U. deningeri*, *U. s. spelaeus* and *U. s. eremus* samples. Significant nonlinear correlations of E2 with L, LPOST and W were found in the sample of *U. kanivetz* (= *ingressus*). The coordinate K1 correlates with L, LANT and indexes IW, ILME. The coordinate K2 correlates with the paracone index, ILPOST and ILANT\_LPOST (Data S4).

The taxonomical composition of sample explains 62.7% of the variance of E1 coordinate of SZM model if *U. arctos*, *U. minimus* and *U. etruscus* are included and 43.5%, if these species are excluded from the analysis. This factor explains 50% of the variance of K1 coordinate (SHM model) in case when *U. arctos*, *U. minimus* and *U. etruscus* are included in the analysis.

In Fig. 4D, the position of the sample centroids within the SZM morphospace is shown. Within the morphospace, three taxa, namely, *U. etruscus*, *U. arctos* and *U. k. kanivetz*, have the largest ranges along both coordinates. Accordingly, they have a higher morphological variability of M1 in comparison with others. *U. k. ingressus* has a relatively high range along the E1 coordinate, but it is distinctly restricted along the E2 coordinate, whereas *U. minimus* has a wide range along E2 only. The centroids of the big cave bears form the group on the right side of the chart. These taxa are characterized by small values of the roundness index (IW) and a high IS proportional to the 'general size' of M1 (Data S4). The next compact group, consisting of *U. k. praekudarensis*, *U. k. kudarensis*, *U. deningeri* and *U. s. ladinicus*, is located to the left of the large group of cave bears. M1 of *U. k. praekudarensis* and *U. deningeri* are similar in all variables, but *U. k. kudarensis* has some wider M1 in relation to previous ones (Data S4). The M1 of *U. s. ladinicus* has practically the same dimensions as the Kudaro bear, but its IW average value (69.7%) is typical for big cave bears (69.1–69.8%). In the Kudaro bear, the roundness index is 73.7–72.2%, which is close to that in Deninger's bear – 72.4%. The centroids of the *U. rossicus* and *U. savini* samples are situated close to each other and not far from the *U. arctos* centroid. In comparison with *U. savini*, the M1 of *U. rossicus* has a relatively short posterior part and an elongated anterior part. *U. rossicus* has an average roundness index of 70.6% (somewhat higher than in big cave bears) and dimensions within the range of the brown bear.

The centroids of *U. minimus* and *U. etruscus* are the most distanced from those of the other studied bears. These two species have the smallest size and the greatest roundness of M1 (IW: 77.9% and 77.5%, respectively). The differentiation between them is substantial due to differences in 'general size' of the tooth. They are differentiated also with respect to the paracone

and metacone indexes (37.7 vs. 40.1% and 37.6 vs. 40.7%, respectively), and the anterior–posterior index (ILANT\_LPOST: 92.8% vs. 88.4%). In other words, in comparison with *U. minimus*, the *U. etruscus* M1 has a larger paracone and metacone and a more elongated caudal part of the tooth.

**M2.** – The dimensionalities of the SZM and SHM morphospaces of M2 were 2 and 3, respectively. The linear regression models, where SZM and SHM coordinates used as independent variables, described the row measures of M2 with coefficients of determination ( $r^2$ ) from 0.81 to 0.97 (Data S4).

The E1 coordinate correlates with all measurements and describes the 'general size' of the tooth (Fig. 4A). As in the cases of P4 and M1, the variability of the index of masticatory surface area is tightly bound to the 'general size' of M2 ( $r = 0.97$ ). The coordinate E2 correlates with the absolute ( $r = 0.75$ ) and relative ( $r = 0.89$ ) length of the metacone; therefore, LME has two independent components of variability. In addition, E2 correlates with the paracone–metacone index ( $r = -0.65$ ).

The coordinates of the SHM morphospace do not show any correlation with the measures of M2, except for K1, which has a weak correlation with WPOST ( $r = 0.58$ ). In addition, it correlates with the metacone index ( $r = -0.74$ ) and anterior–posterior index ( $r = 0.71$ ). Note that nonlinear correlations (cubic regression model was used, Data S4, Fig. S4.1) were observed in all cases. The K2 coordinate has a weak linear correlation with IWPOST ( $r = 0.48$ ) and with paracone–metacone index ( $r = -0.58$ ). The K3 coordinate correlates with the IWANT ( $r = -0.68$ ), IWPOST ( $r = 0.48$ ) and paracone indexes ( $r = 0.52$ ).

The variances of E1 and K1 coordinates are determined by taxonomical composition of the full sample to the extent of about 62% and 33%, respectively.

The ranges of ursid taxa overlap significantly in two-dimensional SZM morphological space (Fig. 5B). The positions of sample centroids within the morphospace mainly reflect differences in 'general size' of M2, from *U. minimus* to *U. k. ingressus*. The group of taxa with largest M2 includes two subspecies of *U. spelaeus*, *U. kanivetz* (= *ingressus*) and both Kudaro bear subspecies. These taxa are differentiated statistically by WPOST, except the subspecies of the Kudaro bear, which have a narrower talon (Data S4). Within the row *U. s. eremus* – *U. s. spelaeus* – *U. k. ingressus*, the width of the talon increases on average. The dimensions and shape of M2 are very similar in *U. s. eremus* and *U. s. spelaeus*. In a pairwise comparison, *U. k. ingressus* and *U. k. kanivetz* revealed differences in the length of the paracone (13.6 vs. 13.1 mm) and more clearly – in the paracone–metacone ratio (121.9 vs. 113.4%). *U. s. spelaeus* differs from *U. k. kanivetz* in the paracone–metacone ratio (121.3%) and from *U. k. ingressus* in the 'general size' of M2, but most clearly in the greater

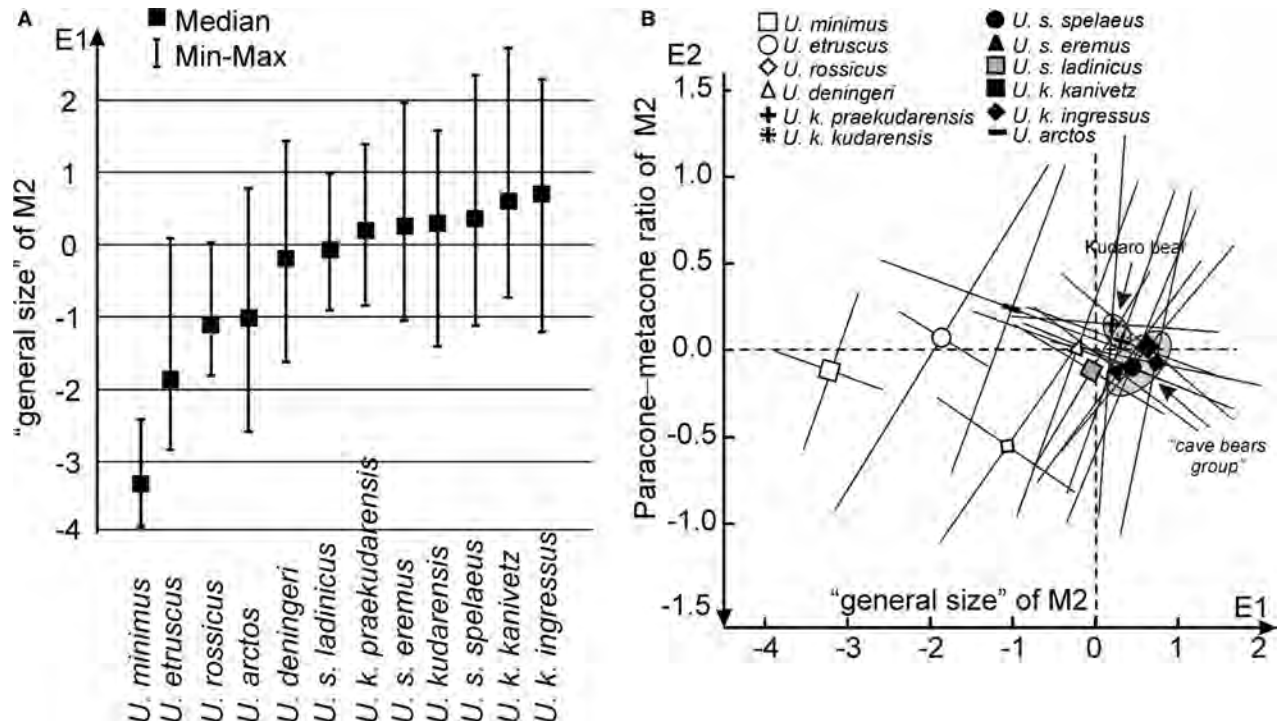


Fig. 5. A. Medians and min-max. of first (E1) coordinate in the bear taxa in SZM morphospaces of M2. B. Centroids and ranges of the bear taxa within SZM morphospaces of M2. Ranges are equal to sample mean (centroid)  $\pm$  highest value – lowest value  $\times 0.95$ .

width of this tooth (22.7 vs. 23.5 mm). The pair of *U. kudarensis praekudarensis* and *U. k. kudarensis* shows a minor difference in the relative width of M2 (50.0 vs. 52.4%; Data S4).

The centroid of *U. s. ladinicus* is situated between the centroids of *U. s. eremus* and *U. deningeri*. *U. s. ladinicus* differs from *U. s. eremus* by the length of M2 (41.8 vs. 43.6 mm) and the length of the paracone (12.0 vs. 12.8 mm). The general dimension of M2 in *U. s. ladinicus* is very close to Deninger's bear on average, but it has relatively wider talon (IWPOST: 47.1 vs. 43.7%).

In the SZM morphospace, the centroid of the small cave bear *U. rossicus* is very far removed from the main cave bear group (Fig. 5B). For this species, an extremely high value of the paracone–metacone ratio (129.2%) is recorded. In comparison with *U. minimus* (ILPA\_LME: 116.4%) and the Etruscan bear (112.3%), this shows a significant reduction of the M2 metacone in *U. rossicus*. Interestingly, a close relationship between the paracone and metacone is recorded in *U. k. ingressus* (121.9%) and *U. s. spelaeus* (121.3%). The most important differences between *U. rossicus* and *U. arctos* are expressed in the general tooth shape and the proportions of its separate parts. The metacone of the small cave bear is shorter than that of the brown bear (8.4 vs. 10.5 mm), the anterior part of the tooth is relatively narrower (IWANT: 49.0 vs. 52.6%), and the talon of M2 is extremely elongated (ILPOST: 51.5 vs. 39.1%). The last-named index is at

its maximum in *U. rossicus* amongst the studied bears. In all other deningeroid–spelaeoid bears, ILPOST varies, on average, from 44 to 46% (Data S4) as opposed to *U. arctos*, *U. etruscus* and *U. minimus* where it is less than 40%. Thus, the talon elongation in M2 is a special property of the cave bear lineage.

The second upper molar of the Etruscan bear occupies an intermediate position between those of *U. minimus* and *U. arctos* within the morphospace (Data S4). The average of L of this tooth (31.7 mm) falls between *U. minimus* (25.0 mm) and *U. arctos* (37.0 mm). The ILPOST index (37.0%) is also intermediate between the last two species (34.6 and 39.1%), the paracone–metacone ratio is somewhat lower (112.3%) than in *U. arctos* (114.6%) and *U. minimus* (116.4%) and it is between those of *U. k. praekudarensis* (111.8%) and *U. s. ladinicus* (112.5%). The relative width values of the *U. etruscus* M2 (IWANT, IWPOST: 56.5, 48.2%) are closer to those of *U. minimus* (58.3%, 51.4%) than to those of *U. arctos* (52.6, 44.3%).

*U. minimus* is the most differentiated taxon because it has the smallest M2 of all the studied taxa. The small size of M2 in this species is associated with several 'primitive' (in comparison with cave bears) features, such as the lowest index of talon length, the highest indexes of metacone and paracone lengths (31.0, 35.0%), and, in addition, the M2 of *U. minimus* has the most rounded contour of the tooth crown (IWANT: 58.3%, IWPOST: 51.4%).

### Basic morphometric trends in cave bear and brown bear lineages

In this section, we present data on variations in cheek teeth at the evolutionary time scale (from the Late Pliocene to the Late Pleistocene) and ecological trends that can be related to the site altitude above sea level (Rabeder et al. 2008, 2010, 2011).

By way of illustration of trends at the evolutionary time scale, three variables that showed significant change amongst the taxa were selected. In the case of the premolar P4, this is the index of masticatory surface area (IS), for the first upper molar M1 – roundness index (IW), and for the second molar M2 – talon length index (ILPOST). The main evolutionary patterns of the selected parameters are shown in Fig. 6. Here we use a logarithmic time scale in order to show the Middle Pleistocene and the Late Pleistocene time intervals in more detail.

Let us first note the insignificant disparity between *U. minimus* and *U. etruscus* against the background of considerable variability between the local samples. Then, the parameters of brown bear teeth are much closer to the parameters of the proposed common ancestor *U. etruscus* than the teeth of representatives of the cave bear lineage. Unfortunately, we cannot demonstrate the transition between *U. etruscus* and *U. arctos* due to the lack of material from the Early Pleistocene of Europe. Since the beginning of the Middle Pleistocene, we can observe characteristics of arctoid bears, which by this time were quite different from *U. etruscus*, at least in the features of P4 and M2.

If the hypothesis of the origin of the deningeroid–spelaeoid lineage from the Etruscan bear is correct, the morphological ‘transition’ *U. etruscus* – *U. deningeri* in Europe (as the material at our disposal is mostly of European provenance) falls at the end of the Early Pleistocene and the Middle Pleistocene. Again, we must pay attention to the gap in information during most of the Early Pleistocene time. Thus, the data do not exclude the possibility of potential immigration of the early Deninger’s bears to western Europe during this time.

According to the morphometric schemes, the Middle Pleistocene European *U. deningeri* can be considered as a ‘transitional taxon’, which occupies an intermediate position between spelaeoid and arctoid lineages. On that background, the morphometric parameters of the teeth in the supposed descendant of Deninger’s bear – the cave bears (*sensu lato*) were relatively stable (again, with variations in the morphometric variables). On average, the cave bears’ parameters remained within the limit of the range in the taxa, which completed the evolution of cave bears (*U. kanivetz = ingressus*) in Europe.

Unlike cave bears, in the brown bear only the ‘general shape’ of the first upper molar, indicated by the IW index, held relatively constant throughout the Middle and Late Pleistocene (as well as the Holocene). The IS index of P4

was stable until the end of the Middle Pleistocene. Then, during MIS 5 – MIS 3 there were brown bears in Europe (*U. a. priscus* Goldfuss, 1818), with P4 reaching the size of the upper premolar of cave bears. At the end of the Late Pleistocene (MIS 2), this tooth reverted to the size that had been observed in the Middle Pleistocene bears or even smaller. Recent geographical populations (subspecies) of the brown bear in Eurasia and North America are characterized by a large variation in their body size. Accordingly, amongst the living bears, the value of the IS index can be at the ‘Middle Pleistocene’ level (large subspecies) or be significantly lower (small-sized subspecies). The relationship of the posterior (talon) and anterior parts of M2 was stable during the Middle–Late Pleistocene time, but after the Last Glacial Maximum (MIS 2), the talon area tends to decrease towards the recent values of the ILPOST index. The evolutionary trends of the IS and ILPOST indexes of brown bear P4 and M2 (Fig. 6) are very similar to changes in the relative length of lower molars in the Pleistocene animals (Kurtén 1968), which correlates with the general body size.

Analysis of samples that include more than three teeth revealed the following trends (based on sample means) in *U. deningeri* in order of descending significance: P4 – increase of relative length of paracone ( $r = 0.64$ ,  $p = 0.01$ ) and a decrease in the number of geographical samples with low roundness index values in the second half of the Middle Pleistocene; M1 – increase in the tooth length ( $r = 0.68$ ,  $p < 0.001$ ), the masticatory surface area index ( $r = 0.64$ ,  $p = 0.002$ ), the length of posterior part of the tooth ( $r = 0.63$ ,  $p = 0.003$ ), the anterior part of the tooth ( $r = 0.53$ ,  $p = 0.01$ ), the paracone area ( $r = 0.49$ ,  $p = 0.02$ ) and the greatest width of the tooth ( $r = 0.56$ ,  $p = 0.009$ ) during the end of Early Pleistocene – the beginning of the Middle Pleistocene; M2 – a decrease in the relative length of the metacone ( $r = -0.43$ ,  $p = 0.07$ ) during the late Early Pleistocene and the beginning of the Middle Pleistocene and an increase in relative length of the talon area (ILPOST,  $r = 0.41$ ,  $p = 0.09$ ) during the same time interval.

No significant morphometric trends were found in P4 of *U. s. spelaeus* during the second half of the Late Pleistocene. Perhaps the change in this tooth occurred earlier, at the end of the Middle Pleistocene and in the first half of the Late Pleistocene. The trends detected in M1 are nonlinear as the changes took place during a relatively short time interval, approximately between 60 and 45 (40) ka BP, and they include: the increasing of the posterior part of the tooth ( $r = 0.63$ ,  $p = 0.004$ ), IS index ( $r = 0.62$ ,  $p = 0.005$ ), the paracone length ( $r = 0.59$ ,  $p = 0.008$ ), the greatest length ( $r = 0.56$ ,  $p = 0.01$ ) and width ( $r = 0.55$ ,  $p = 0.01$ ) of the tooth, the relative length of the posterior part of the tooth ( $r = 0.51$ ,  $p = 0.03$ ), a decrease in the ratio between paracone and metacone lengths ( $r = -0.50$ ,  $p = 0.03$ ). In contrast to M1, the second molar M2 underwent changes closer to the end of the Late Pleistocene, approximately from 40 (45) ka BP

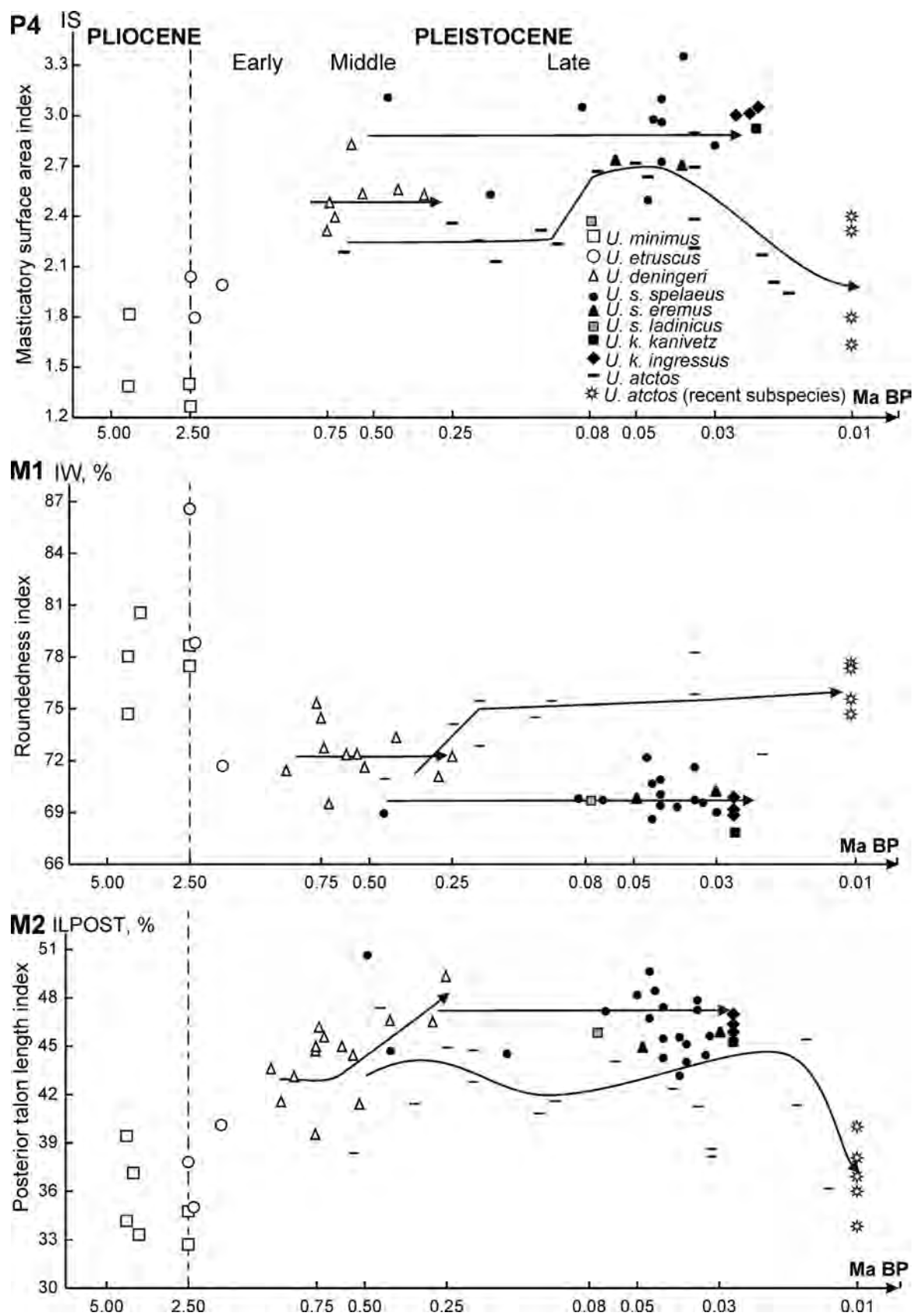


Fig. 6. Evolutionary trends of the IS, IW and ILPOST indices in spelaeoid and arctoid lineages in the Pleistocene of Europe.

to the Late Glacial Maximum. These morphometric trends were expressed as follows: increase in the length of paracone ( $r = 0.68, p < 0.001$ ), the general length of the tooth ( $r = 0.52, p = 0.01$ ) and the IS index ( $r = 0.52, p = 0.01$ ), the greatest width ( $r = 0.50, p = 0.02$ ) and the width of the talon area ( $r = 0.46, p = 0.03$ ) in the youngest localities. The scant data (several teeth from six sites) recovered from the Middle Pleistocene localities do not allow conclusions about the absence or presence of directed changes in the second molar structure. It is possible that within the MIS 13–MIS 6 time interval, no significant changes took place in the dimensions of this tooth.

We could not detect any direct changes in the size and shape of the upper premolar P4 in the Kudaro bear. The M1 of the Middle Pleistocene subspecies (0.70–0.25 Ma BP), *U. k. praekudarensis*, shows a more or less linear tendency to decrease in tooth size, which is especially clearly expressed in its greatest width and relative width ( $r = -0.93, p = 0.006$ ;  $r = -0.91, p = 0.01$ ), the length of the posterior part ( $r = -0.93, p = 0.007$ ) and the length of the anterior part ( $r = -0.81, p = 0.05$ ). In this case, there was an allometry between changes in the protocone and the metacone in such a way that their ratio increased ( $r = 0.85, p = 0.03$ ). This tooth in the Late Pleistocene subspecies *U. k. kudarensis* (0.09–0.025 Ma BP) showed the opposite trend in its changes, including increase in the tooth width ( $r = 0.60, p = 0.07$ ) and, probably, in the length of the anterior part and the length of the paracone. Technically, these are only tendencies, insofar as no statistically significant correlations with the age of localities have been obtained. Against this background, the tooth shape did not change. Finally, the available data do not allow a definite conclusion on the M2 of the Kudaro cave bear decreasing or increasing during the Middle–Late Pleistocene.

In addition, the effect of altitude on the teeth measures and indexes was tested. The roundness index of P4 correlates with elevation above sea level of the locality in *U. deningeri*, *U. s. spelaeus* and *U. arctos*. For *U. kanivetz ingressus* and *U. k. kanivetz* the altitude correlates with P4 length (Table 3). The roundness index of M1 changes with the altitude value in the brown bear only. The paracone index shows correlation with the altitude in M1 of *U. deningeri* and in M2 of *U. arctos*. The

metacone length of M1 varies with altitude in *U. k. kanivetz*, and the ILPOST index of M2 shows correlation in *U. arctos*.

According to these results, parameters of P4 are most sensitive to ecological and physical factors that can be associated with altitude.

### Morphological diversity

Morphospace dimensionalities ( $d$ ), calibrated entropy ( $H$ ) and orderliness/redundancy ( $R$ ) calculated for the SZM models (size diversity) and SHM models (shape diversity) for all the studied taxa are presented in Table 4. Based on these results, we must reject the null hypothesis that the morphological diversity is equal for all upper cheek teeth in bears because the diversity of the M1 is significantly lower and orderliness is higher than diversity/orderliness of the premolar and the second molar. In this case, as is typical for bears, M1 is noticeably smaller than M2, which cannot be explained by the inhibitory cascading model (see Asahara *et al.* 2016) if this model is extrapolated from the lower molars to the upper ones. The low diversity of M1 is implemented at the species level especially for standardized entropy ( $H/d$ ) and for the diversity of the tooth general size (Fig. 7, Data S5).

By the sum of the standardized entropy values, which characterize both size and shape diversity, the brown bear and Deninger's bear have the greatest morphometric diversity (the lowest parameter  $R$ , accordingly) of all the teeth overall. The lowest diversity is observed in the final taxon of the cave bear lineage – *U. kanivetz (=ingressus)*. The comparison of the morphological diversity between the Deninger's bear and the Kudaro bear has shown that it is generally higher in the first species (Fig. 7).

At the subspecies level, the orderliness ( $R$ ) of M1 usually is higher in comparison with P4 and M2 (Fig. 7, Data S5), but as to the size diversity, it is lower or close to the orderliness of P4 (*U. s. ladanicus*, *U. k. kanivetz*) or M2 (*U. s. spelaeus*, *U. k. ingressus*). The diversity of P4 is high in all bears except the sample of *U. s. ladanicus*.

Between the two subspecies of *U. kudarensis*, the size diversity of P4 is higher in the Middle Pleistocene *U. k. praekudarensis*; the size diversity of M1 and M2

Table 3. The correlations between selected teeth features and the altitude of sites.

Taxon	P4		M1			M2	
	IW	L	IW	ILPA	LME	ILPA	ILPOST
<i>U. deningeri</i>	$-0.78, p < 0.01$	–	–	$0.69, p = 0.003$	–	–	–
<i>U. s. spelaeus</i>	$-0.78, p < 0.01$	–	–	–	–	–	–
<i>U. k. ingressus</i>	–	$-0.52, p = 0.08$	–	–	–	–	–
<i>U. k. kanivetz</i>	–	$-0.95, p = 0.04$	–	–	$0.93, p = 0.06$	–	–
<i>U. arctos</i>	$-0.76, p = 0.01$	–	$0.79, p = 0.02$	–	–	$0.64, p = 0.03$	$-0.59, p = 0.45$

Table 4. Morphospace dimensionality ( $d$ ), calibrated entropy ( $H$ ), redundancy/orderliness ( $R$ ) and their 95% confidence intervals.

Tooth	Size diversity					Shape diversity				
	$d$	$H$	95% interval	$R$	95% interval	$d$	$H$	95% interval	$R$	95% interval
P4	2	4.27	4.16–4.36	0.203	0.223–0.184	3	6.25	6.11–6.37	0.047	0.065–0.032
M1	2	2.39	2.28–2.49	0.539	0.559–0.519	2	2.63	2.52–2.74	0.492	0.513–0.470
M2	2	5.48	2.95–3.14	0.124	0.142–0.106	3	4.62	4.48–4.77	0.237	0.256–0.218

is similar in both subspecies, and the shape diversity of these teeth is higher in the Late Pleistocene *U. k. kudarensis* (Fig. 7).

The orderliness of P4 and M2 size diversity shows some multidirectional correlation ( $r = 0.76$ ,  $p = 0.017$ ;  $r = -0.62$ ,  $p = 0.08$ ) with environmental factors expressed in elevation above sea level amongst several Late Pleistocene *U. spelaeus* and *U. kanivetz* (= *ingressus*) local populations.

On average, the described pattern for the standardized entropy and orderliness is also observed at the local sample level (Data S5), but concurrently many local samples deviate from this ‘rule’. For example, in the Odessa-Nerubaj caves and Il’inka samples (*U. k. ingressus*, Ukraine), orderliness ( $R$ ) of M1 size diversity (0.25 and 0.22) is higher than of P4 (0.22, 0.19) and M2 (0.17, 0.21), but in the Gamssulzenhöhle (*U. k. ingressus*, Austria) sample, the opposite situation is observed ( $R$ : P4 – 0.22, M1 – 0.16, M2 – 0.24). Amongst the three *U. deningeri* samples, the  $R$  is higher for M1 in the Koněprusy sample only (P4 – 0.22, M1 – 0.29, M2 – 0.21), while in the other two samples (Mosbach and Westbury-Sub-Mendip), the redundancy of M1 was lower at least than that of P4.

#### Multivariate allometry and its interpretation

An allometry pattern provides the statistical relationship between the size and shape of a tooth. In this section, we focus on this problem and consider it in the context of evolutionary allometry.

The proportion of total variance of P4 measurements accounted for by the ‘general principal component’ (GPC1) is 86.7% (95% confidence interval – 85.2–87.9). GPC1 describes the ‘average’ pattern of size variation of a tooth in all taxa simultaneously. The MACs (Table 5) reflect the allometry pattern, which is close to isometry for L, LP and  $R$  measurements, or weak negative allometry – for W. The particular specific PC1s deviate from the GPC1 ‘baseline’ at different angles (Fig. 8). The angles between PC1 and GPC1 in *U. minimus* and *U. etruscus* are about 27.56° and 24.35°, respectively. The peculiarity of the *U. minimus* allometric pattern is shown in the combination of a rather pronounced positive allometry in the lengths of the tooth (MAC: 1.23) and paracone (1.19) with the practical absence of allometry variation of tooth width (0.154; it is notable that *U. minimus* has the lowest roundness index amongst

the studied taxa; Data S6). This means that in this potential ancestral species the length and width of P4 varied relatively independently from each other. In contrast to *U. minimus*, the Etruscan bear’s P4 has values of MACs for L and LP that are indicative of a negative allometry, while the W and  $R$  values suggest a weak positive allometry.

The angle between PC1 and GPC1 in *U. deningeri* (joint sample of Koněprusy, Einhornhöhle, Mosbach and Westbury-Sub-Mendip localities) is 25.19°. The Deninger’s bear allometric pattern is characterized by a more pronounced positive allometry of  $R$ . The PC1 of *U. spelaeus* deviates from the ‘baseline’ by 27.8°. The allometric pattern in this cave bear is similar to the pattern of *U. etruscus*. The angle between the ‘baseline’ and PC1 of *U. kanivetz* (= *ingressus*) (joint sample of Odessa-Nerubaj caves, Il’inka, Gamssulzenhöhle, Nietoperzowa cave and Secrets cave) is about 29.3°. This taxon has negative allometry, especially that of the paracone (0.79), and a strong positive allometry (1.35) in the protocone area. In other words, with an increase in the general tooth size, the measure that correlates with the protocone complex size ( $R$ ) increases faster than the paracone one and then the greatest length of the tooth. This character distinguishes this cave bear significantly from the other taxa. The PC1 of *U. rossicus* deviates from the ‘baseline’ by 39.23°. The allometric pattern of *U. rossicus* is characterized by negative allometry of L and LP, close to isometry of W, and positive allometry of the protocone complex size ( $R$ ). The allometric pattern of this species is closest to the brown bear pattern (Fig. 8). The pattern of the Kudaro bear lineage is very close to the *U. deningeri* pattern, and its PC1 deviates from the GPC1 by 27.45°. The angle between the PC1 and GPC1 in *U. arctos* (joint sample of Biache-Saint-Vaast and Taubach Pleistocene localities and recent subspecies) is very small at ~5.3° and, overall, the brown bear P4 has the most isometric pattern of allometry according to the MAC values (Data S6).

The M1 GPC1 accounts for about 81.2% of variance out of the total variance of all ursid taxa, but in this case, the bootstrap 95% confidence interval was 81.5–84.0% when *U. minimus* data were excluded, and 6.1–82.4% when they were included in the PCA. The wide last interval means that M1 in *U. minimus* has not only a very small tooth size, but also a peculiar covariance matrix in comparison with all other taxa. This leads to instability of the general covariance matrix and to a broad confi-

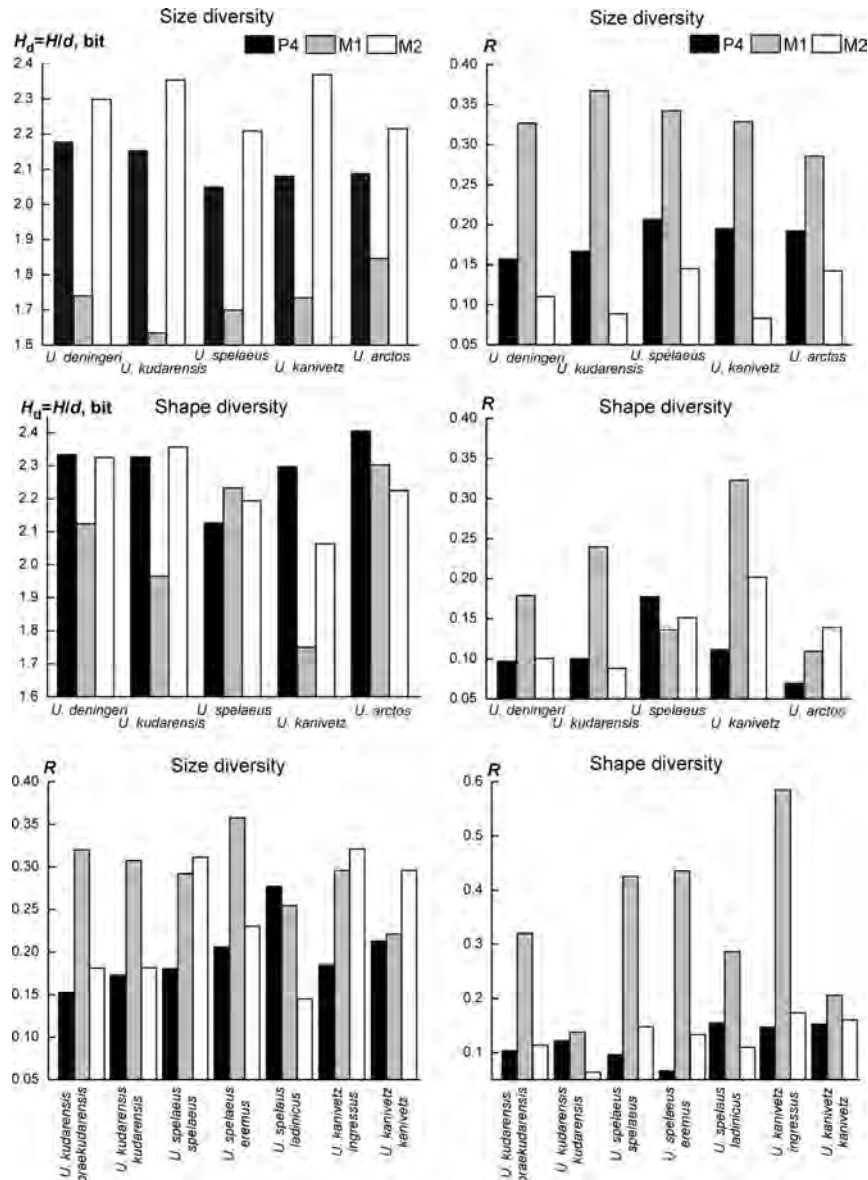


Fig. 7. Parameters of size and shape diversity of the cheek teeth (P4, M1 and M2):  $H_d$  = standardized entropy ( $H/d$ );  $R$  = redundancy/orderliness.

Table 5. Allometric coefficients (MACs and bootstrapped 95% confidence intervals) for the upper cheek teeth in the studied ursids. PCA models include all taxa.

Tooth	L	LP	W	R		
P4	1.005 1.004–1.006	1.084 1.083–1.085	0.903 0.902–0.904	0.998 0.997–0.999		
	L	LANT	LPOST	LPA	LME	W
M1	1.066 1.064–1.068	1.069 1.067–1.072	1.135 1.132–1.137	1.013 1.01–1.016	0.827 0.822–0.831	0.849 0.847–0.852
	L	LPA	LME	WANT	WPOST	
M2	1.079 1.076–1.082	0.852 0.847–0.857	0.887 0.878–0.895	0.987 0.985–0.989	1.159 1.155–1.164	

dence interval for the percent of total variance explained by the GPC1. Nevertheless, there is a well-pronounced general pattern of M1 size variation for other taxa. The ‘average’ allometric pattern of M1 is close to weak positive allometry for L, LANT and LPA, a more pronounced positive allometry in LPOST and a moderate negative allometry for LME and W (Table 5). The positive allometry of the length of the posterior part of M1 directly indicates the relative dominance of it in relation to the anterior part of this teeth.

The angle between the ‘baseline’ and *U. minimus* PC1 is 40.9° (Fig. 8). Amongst the unique features of this allometric pattern (Data S6), noteworthy is the lack of allometry in the length of the paracone and a very weak positive allometry in the length of the metacone and its width. The angle between the PC1s of *U. minimus* and the Etruscan bear is 35.4°. The angle between GPC1 and *U. etruscus* PC1 is smaller (about 10°), and the MACs provide negative allometry for L, LPOST and LME, or approximate isometry for LANT and LPA.

The angle between the *U. deningeri* PC1 and the ‘baseline’ is 28.6°; all MACs vary from a weak negative to positive allometry (MAC: 0.96–1.06). The allometric pattern is similar to that in *U. kudarensis*, but the angle between their PC1s is large (about 23.8°). The PC1 of the Kudaro bear deviates from the ‘baseline’ by 44.5°, i.e. more noticeable in comparison with Deninger’s bear. The allometry varies from weak negative (L, LANT, LPA, W) and isometric (LPOST) to weak positive (LME).

The PC1 of *U. spelaeus* s. str. (Zoolithen cave, Goyet 5B, Furtins, Arcy-sur-Cure and Cova Eirós) deviates from the ‘baseline’ by 37.3°. The allometric pattern in this cave bear is similar to the pattern of *U. kanivetz* (= *ingressus*) (joint sample of Odessa-Nerubaj caves, Il’inka, Gamssulzenhöhle, Wierzchowska cave, Buteshty 1, Secrets cave and Medvezh’ya cave). The angle between the two PC1s is very small – 0.60°. However, *U. spelaeus* s. str. shows more pronounced negative allometry in the length of the anterior part and positive allometry in that of the posterior part of M1 (Data S6).

The small cave bear’s PC1 deviates from the ‘baseline’ by an extremely large angle – 59.2°. The allometric pattern of M1 is very peculiar in this species (Data S6). There is negative allometry (MAC: 0.86) in the anterior part, length of paracone, and length of tooth as a whole. In contrast, the posterior part and length of the metacone have significant positive allometry (1.01, 1.17), and the greatest width of M1 shows isometry (0.93).

The PC1 in *U. arctos* (joint sample from Torn Newton cave, Biache-Saint-Vaast, Taubach, Nizhneudinskaya cave and recent subspecies) is relatively closest to the ‘baseline’ (the angle is 18.6°), except for the Etruscan bear. Noteworthy is an unusual combination of pronounced negative allometry of the paracone and metacone area lengths (MAC: 0.85, 0.69) with positive allometry for the length of the anterior part of M1 (1.15).

The M2 GPC1 explains about 72% only (95% confidence interval: 69.5–74.2%) of the total variance within all ursid species. In this case, the next principal component accounts for about 17.3% of the total variance. In general, it is reflected in a significant dispersion of points on the scatterplot (Fig. 8). For M2, the ‘average’ allometric pattern combines isometry or close to it in variations of the maximum length (L) and greatest width of the tooth (WANT) on the one hand with weak negative allometry for the paracone (LPA) and metacone (LME) lengths on the other (Table 5). An important role in this pattern plays the positive allometry of WPOST.

The allometric pattern in *U. minimus* differs markedly from the ‘average’ pattern as described above. Firstly, there is strong negative allometry of the general length (MAC: 0.77) and length of paracone (0.71) and, secondary, positive allometry in the metacone length (1.19). On this background, the M2 width varies almost isometrically in the anterior and posterior parts. The angle between the ‘baseline’ and the *U. minimus* PC1 is 24.3° (Fig. 8), which is much smaller than in the case of M1. The angle between PC1s of *U. minimus* and *U. etruscus* is 25.5°. The angle between PC1s of *U. minimus* and *U. deningeri* is 2.7° and between PC1s of *U. minimus* and *U. rossicus* is 40.8°.

The angle between the ‘baseline’ and the *U. etruscus* PC1 is very small (about 1.6°), but regardless of that, the allometric pattern in the Etruscan bear is far from the ‘average’ one: it presents a unique combination of strong positive allometry in the paracone–metacone area (MAC: 1.33, 1.23) with strong negative allometry for the other measurements of this tooth (0.58–0.79).

The angle between the *U. deningeri* PC1 and the ‘baseline’ is 26.4°. The specific allometric pattern includes isometry of the paracone length, strong positive allometry of the metacone length and negative allometry for the other measurements. This pattern is close to the *U. kudarensis* pattern, and the PC1s of the Deninger’s and Kudaro bears form an angle of 10.7°. The PC1 of the Kudaro bear deviates from the ‘baseline’ by 36.7°. The allometry has a unique feature – MAC for the talon complex is close to 0 (allometry is absent). In addition, there are very low allometric coefficients in the M2 largest length and width in the anterior part.

The PC1 of *U. spelaeus* s. str. deviates from the ‘baseline’ by 32.1°. The allometric pattern in this cave bear is similar to the pattern in *U. kanivetz* (= *ingressus*) (Data S6). In this case, a difference between the taxa is observed in the width of the posterior part of the tooth, where *U. spelaeus* has stronger negative allometry. The angle between the *U. spelaeus* and *U. kanivetz* (= *ingressus*) PC1s is very small, 6.7°.

The PC1 of *U. rossicus* deviates greatly from the ‘baseline’ (by an angle of 52.7°). The allometric pattern of M2 is very peculiar in this species. There is strong negative allometry of all the measurements except LPA,

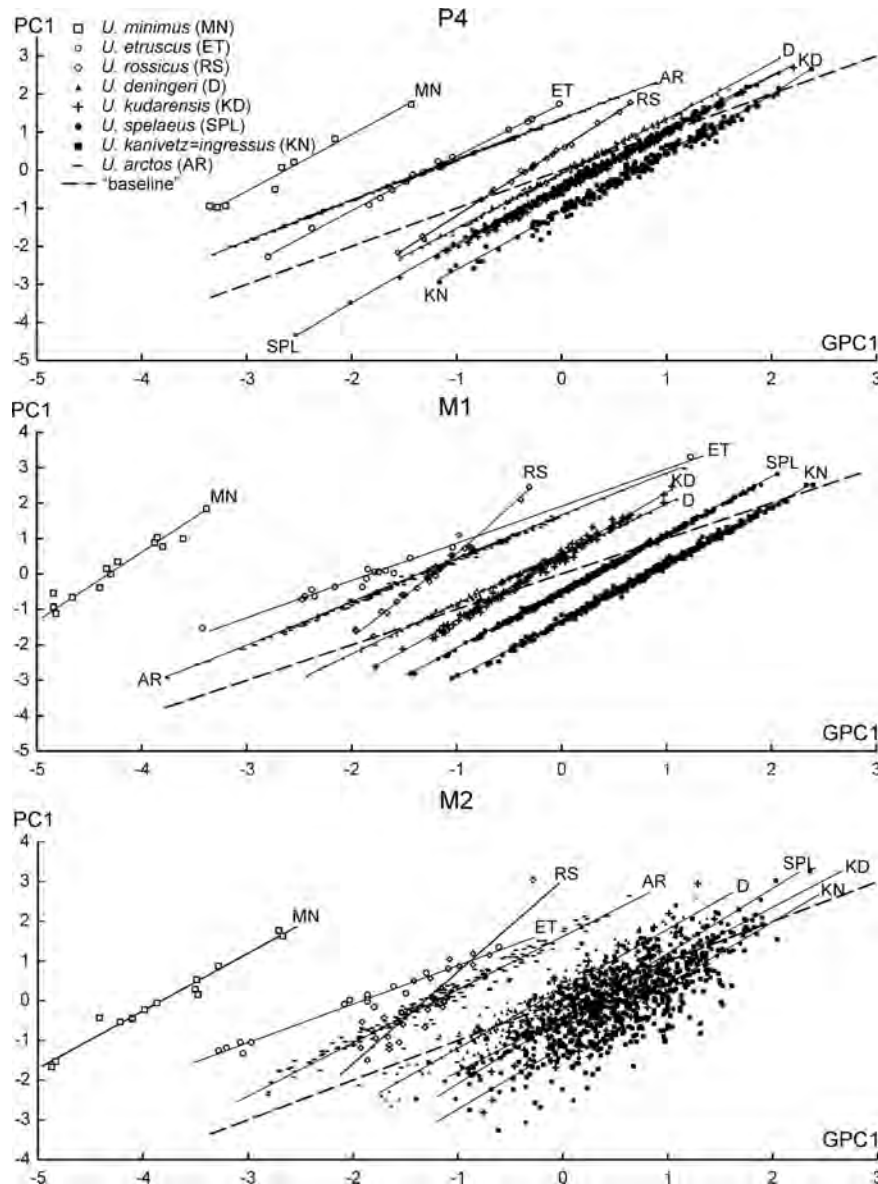


Fig. 8. The P4 – M2 allometric patterns (PC1) of several bear taxa in relation to the 'baseline' pattern calculated for the full set of taxa (GPC1).

the variation of the latter weakly depending on M2 general size (MAC: 0.30).

The brown bear's PC1 (joint sample of Biache-Saint-Vaast, Taubach, and recent subspecies) is closer to the 'baseline' (the angle is  $15.7^\circ$ ) than that of the previous taxon. The allometric pattern of this species includes isometric variation of L, LME and WANT, weak positive allometry in WPOST and negative allometry in the paracone length.

The considered data allow us to conclude that the general allometric pattern of tooth variability is more or less stable in all examined taxa. This pattern was reproduced by the first principal component in the PCA (as well as the first coordinate of the SZM morphospace). The deviations from the common allo-

metric pattern characterize the variants in the covariance matrix at the species and subspecies levels and they are particularly well pronounced in local chrono-populations (see Data S6 for more details). The allometries of P4, M1 and M2 are not strictly synchronized. This is reflected, for example, in the variability in the allometric patterns of the paracone and metacone, which are specific for each tooth. In addition, closely similar patterns are found in different species or even in local populations, which may indicate a high probability of parallelisms in evolution based on tooth ontogenesis regulation constraints shared between all studied bears.

Against the backdrop of the variety of allometric relationships between parts of the teeth, in a number of cases we discovered limitations that could contain a

phylogenetic signal. Two types of variables, the angles between PC1s and MACs, provide information about changes in the tooth shape in a broad sense. Below, we have used them to classify species and subspecies of bears.

The classification based on MACs (Fig. 9A) includes information obtained from all the teeth. In the NJ tree the brown bear, Etruscan bear and small cave bear are well differentiated from the big cave bear group, while cave bears are divided into two sub-clusters including, first, Deninger's bear with the Kudaro bear, and, second, *U. spelaeus* with *U. kanivetzi* (= *ingressus*). Intraspecific differentiation based on allometric patterns well represents the phylogenetic signal in all cases. The classification of species and subspecies based on the angles between specific PC1s gave a similar result (Data S6).

#### Morphometrical classifications and phylogenetic signals

The coordinates of the taxon centroids in all the modelled SZM and SHM morphospaces of P4, M1 and M2 were used for classification, which aggregates data collected on all three teeth (Fig. 9B, C; for more details see Data S7). The variation in the general size of teeth strongly influences the structure of the tree. An increase in masticatory surface area is considered as an evolutionary adaptation to omnivore or herbivore diets in the spelaeoid lineage. The practically linear correlations between the index of the masticatory surface (IS) and the linear dimensions of teeth 'mark the possible way to achieve these adaptations'. Note, here we do not consider the complication of the surface morphology, which occurred usually in parallel with the increase in the teeth size (Rabeder & Tsoukala 1990).

In relation to general size and chewing surface area, the studied taxa form practically continuous series on the NJ tree, from the smallest *U. minimus* to the largest subspecies of *U. kanivetzi* (= *ingressus*). There are only two more or less compact clusters: a cluster of the Kudaro bear (the genetically separate lineage) and a fuzzier cluster of big cave bears. The relationships within the latter are also dependent on the general size of teeth: the taxa are ordered in a row from the relatively medium-sized *U. s. ladinicus* via the largest subspecies of *U. s. spelaeus* to the final forms in the evolution of cave bears – *U. k. kanivetzi* (northeast of Europe) and *U. k. ingressus* (central, southern and southeastern Europe).

The split of the subspecies of the Kudaro bear and Deninger's bear has good bootstrap support on the NJ tree, conforming to the hypothesis about the parallel evolution of *U. deningeri* and *U. kudarensis*.

The small cave bear (*U. rossicus*) is placed between the *U. arctos* and *U. deningeri* branches on the NJ tree.

#### Discussion

A multivariate analysis of the upper cheek teeth showed a significant overlap of the size/shape parameter ranges in

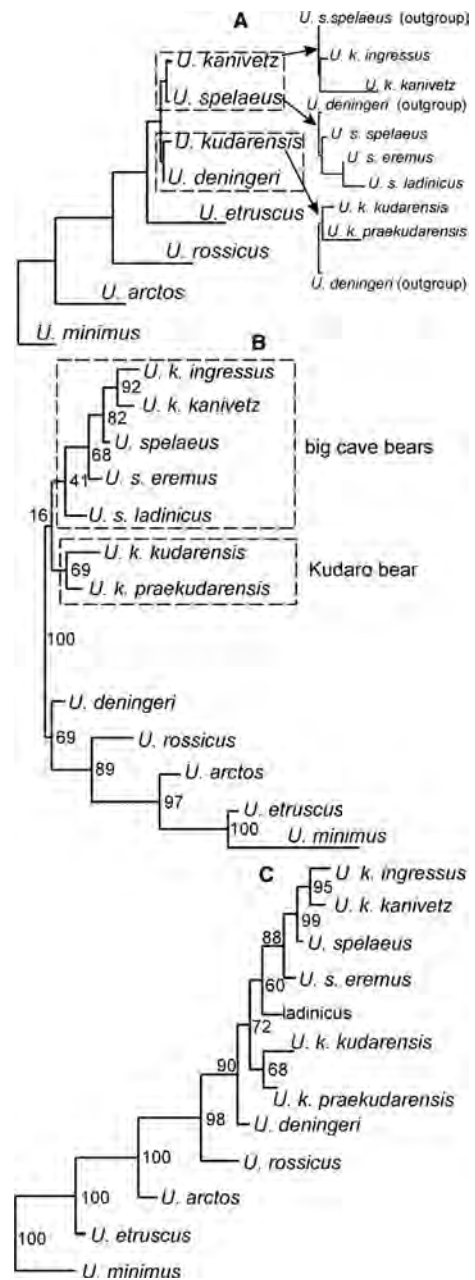


Fig. 9. A. The neighbour-joining tree of taxa (species and subspecies separately) based on MACs of all the upper cheek teeth (Euclidean distance used). B, C. The neighbour-joining tree (rooted on the last branch added during tree construction (A) and rooted on *U. minimus* (C); Euclidean distance used in both cases) based on coordinates of species or subspecies centroids in all SZM and SHM morphospaces of P4, M1 and M2. Bootstrap support values (%; 1000 repeats) are shown at the branch nodes.

deningeroid and spelaeoid bears (*U. deningeri*, *U. kudarensis*, *U. rossicus*, *U. spelaeus*, *U. kanivetzi* (= *ingressus*)), as has been previously shown for the skull and metapodial bones in studies including large samples of bear remains from numerous geographical locations (Baryshnikov & Puzachenko 2011, 2017). The ranges of

potential ancestral taxa (*U. minimus*, *U. etruscus*) and the brown bear (*U. arctos*) also overlap significantly with the cave bear range within morphological space.

Against this background, the morphospace models constructed here allowed us to trace the evolutionary changes that have some specific characteristics for the different teeth as well as common features. The latter include an increase in tooth size and an allometric increase of their chewing surface, which reaches the maximum in big cave bears. In the first and second molars (M1 and M2), the length increases to a greater extent than the width of these teeth, which manifests itself in the general fall in the roundness index (IW) in the row from *U. minimus* to the cave bears.

The evolution of the premolar P4 is more specific. The value of the roundness index for this tooth that is typical of cave bears was reached already at the evolutionary level of the Etruscan bear. The further increase in the premolar size in cave bears was brought about by a proportional increase in both the length and the width of this tooth. During the evolution of the brown bear and the Kudaro bear (transition from *U. k. praekudarensis* to *U. k. kudarensis*), both the length and width of P4 increased in parallel, resulting in greater roundness of the premolars. This happens in both cases due to the increase in the shortest distance between the frontal ridge of the protocone and the posterior side of P4. This example shows the possibility of independent evolutionary transformation in separate ursid lineages, with equivalent effects.

The centroids of the cave bear subspecies form a compact group in the modelled morphospaces except for the smallest subspecies *U. s. ladinicus*. This group is separated from the *U. deningeri* centroid, *U. rossicus* centroid and the centroids of the Kudaro bear subspecies within the size diversity model (SZM). All subspecies of *U. spelaeus* and *U. kanivetz* (= *ingressus*) have close morphometric parameters describing the variability of teeth proportions (indices), but mainly differ from each other in the general dimensions of the teeth.

On average, the greatest distances between centroids are observed in the models describing variations in the tooth sizes (Table 6). Of the three teeth considered in the cave bear group, the greatest distance between centroids is observed in the P4 morphospace. Thus, P4 is potentially most useful of the three teeth in studying the

morphological differences between the cave bear subspecies. The premolar also displays maximal difference in the subspecies of the Kudaro bear (Table 6). In this case, however, variations in the shape of teeth are more important than changes in their size.

In the morphological differentiation of *U. minimus*, *U. etruscus*, *U. arctos* and *U. deningeri*, the variability in M2 size and the M1 shape are of great importance. Most likely, these evolutionary changes in the upper molars occurred asynchronously as the differentiation reflects the early successive stages of evolution. Based on the results of this study, we assume the following sequence of evolutionary transformations in the upper cheek teeth in the studied species. The pair *U. minimus* – *U. etruscus* diverged in the dimensions of M2, and to a much greater extent in the shape of M1 and P4. The divergence of *U. etruscus* and *U. arctos* affected the shape and size of M2 and the shape of P4 first, and only secondarily the dimensions and shape of M1. The extent of the morphological divergence between the Etruscan bear and European Deninger's bear is much greater than between the former and the brown bear. The main contributions were made by changes in M2 size, then in the size and shape of M1 and finally in the size of P4. The proposed evolution from Deninger's bear to the cave bear (taking *U. s. spelaeus* as an example) affected mainly the dimensions of all three teeth (especially M2), and the shape of P4. The changes in the premolar were the most significant overall. In this context, it should be noted that a gradual complication in the morphological structure of P4 (expressed in morphodynamic indices (Rabeder & Tsoukala 1990)) most clearly marks the final stages of the evolution of the cave bear lineage. The main variations in the morphometric parameters of P4 are shown in Fig. 10 (see also Data S7).

The morphological disparities between the studied cave bear subspecies, the Kudaro bear and Deninger's bear, as illustrated in the NJ trees (Fig. 9), are in good correspondence with the distances in schemes of genetic differentiation based on ancient mitochondrial DNA (Valdiosera et al. 2006; Dabney et al. 2013; Stiller et al. 2014). In general, the phylogenetic signal is more pronounced in the variability of teeth in comparison with other skeletal remains of cave bears (cranium, mandible, or metapodial bones).

Table 6. Standardized Euclidean distances ( $D/d$ , where  $d$  = morphospace dimensionality) between centroids of cave bear subspecies (*U. spelaeus*, *U. kanivetz* (= *ingressus*)), Kudaro bear subspecies and the other taxa of bears in the SZM and SHM morphospaces of P4, M1 and M2 cheek teeth.

Morphospace	Cave bear subspecies				Kudaro bear subspecies				<i>U. minimus</i> , <i>U. etruscus</i> , <i>U. arctos</i> , <i>U. deningeri</i>			
	P4	M1	M2	Sum	P4	M1	M2	Sum	P4	M1	M2	Sum
SZM	0.25	0.23	0.20	0.68	0.13	0.10	0.07	0.30	0.56	0.51	0.71	1.77
SHM	0.11	0.09	0.09	0.30	0.17	0.15	0.11	0.43	0.21	0.62	0.32	1.14
Sum	0.36	0.32	0.29		0.30	0.25	0.18		0.77	1.12	1.03	

However, there is a mismatch amongst the morphological, phylogenetic and genetic classifications for the small cave bear. Based on mitochondrial evidence, *U. rossicus* from the Kizel Cave (Ural region, Russia) should be placed within the lineage of the ‘*ingressus*’ haplogroup (Stiller et al. 2014). In the phylogenetic scheme by Rabeder et al. (2010) the divergence of *U. rossicus* is placed between the ‘*U. etruscus* group’ and the ‘*U. deningeri* group’, after the divergence of the Kudaro bear. The position of *U. rossicus* between *U. arctos* and *U. deningeri* on the NJ tree in this paper (Fig. 9) is not unexpected in the light of the results obtained from our previous studies. The morphometrical parameters of both the cranium and mandible bone of this species are close to those in the brown bear (Baryshnikov & Puzachenko 2011) or occupy an intermediate position between Deninger’s and brown bears (Baryshnikov and Puzachenko 2018). *U. rossicus* is also notably different from other spelaeoid bears in the size of metapodial bones (Baryshnikov & Puzachenko 2017). Herewith, the shape of the metapodial bones has all the key characteristic features of big cave bears. The M1 shows unique features in *U. rossicus* such as a high ILANT index with the combination of low paracone, metacone and surface area (IS) indices (the latter is similar to that in the brown bear), and a roundness index that is higher than in other cave bears. The second molar is characterized by the lowest roundness index amongst all of the studied taxa and the highest paracone–metacone index. In addition, the small cave bear is close to *U. s. ladinicus* in the parameters of P4. Overall, the unique combination of the morphological features of the teeth differentiates this taxon sharply from Deninger’s

bear and the big cave bear group, including *U. kanivetzi* (= *ingressus*).

We first applied the multivariate allometry approach (Cock 1966; Klingenberg 1996), including MAC and the angles between PC1, to investigate teeth variability in cave bears. The results of our work show that variation in both the MAC and in the angles between the GPC1 and specific PC1s may contain a phylogenetic signal and reflect the evolution of allometry (in *U. deningeri* for example). Studies of multivariate allometry make it possible to better understand coordinated changes in different parts of the tooth and to obtain a generalized assessment of the differences between taxa or even between separate chrono-populations. Thus, we believe that these variables are quite suitable and useful for studying the morphological variability of palaeontological material.

Two types of morphological space allow separate investigation of the size and shape diversity. These statistical models allow information-theoretical parameters to be used for estimating tooth diversity – entropy (not only its Shannon variant in the general case) and orderliness. First, it was proposed (as a ‘null hypothesis’) that there is no difference in the morphometric diversity of upper cheek teeth in the studied bear taxa. The null hypothesis was rejected because of greater orderliness in the first molar M1 diversity as compared with the premolar and second molar for the full sample (includes all taxa) and at the species level. At least two phenomena can be hidden there. First, it can be a narrow range of M1 variability due to various constraints, from genetic control to mechanical restrictions imposed by the adjacent teeth. For example, in many voles (Arvicolinae, Rodentia), the molars (M3, m1) on the edge of the tooth row are usually characterized by high morphological variability. However, in mammalian ontogeny, m1 affects the development of m2 and not vice versa, according to inhibitory dynamics of molar initiation (Kavanagh et al. 2007). Therefore, the hypothesis of ‘suppression’ of M1 diversity by neighbouring teeth in bears lacks support. This is not surprising, as the basic model does not describe the ratio amongst the lengths of the lower teeth in bears or in horse and vole species (Asahara et al. 2016). We hope to return to studying this problem after analysing the data on the lower cheek teeth.

Another, but not an alternative, mechanism that could explain the low diversity of this tooth is the possibility of asynchronous evolutionary transformation in different teeth. The important role of M1 parameter changes was shown for divergence at the species level (*U. minimus* – *U. etruscus*, deningeroid bears – cave bears). However, the role of M1 in morphological differentiation at the intraspecific level was significantly lower. Thus, at the species level the low morphometric diversity of the first molar reflects the fixation of different morphological variants in different species on the background of the relatively high diversity in P4 and M2. An indirect

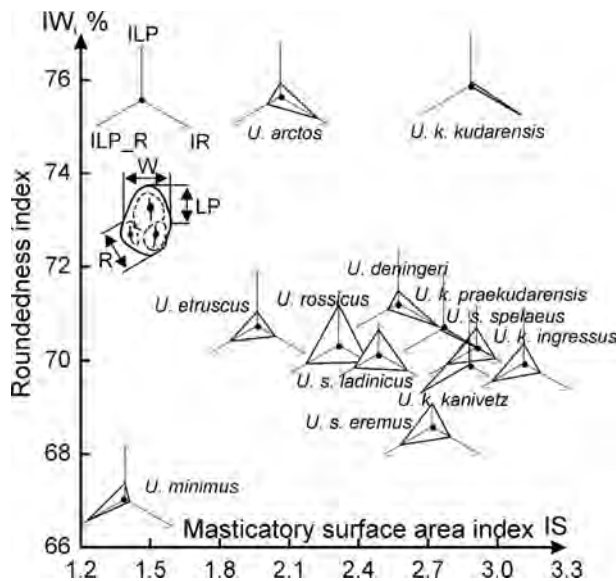


Fig. 10. Morphological variations in P4 amongst cave bears, Kudaro bear, and their probable ancestors. Abbreviations as in Fig. 3.

confirmation of this follows from the absence of altitude effects upon the M1 diversity in *U. spelaeus* and *U. kanivetz* (= *ingressus*). Another indirect confirmation of differences in the genetic and epigenetic regulation of the teeth parameters is associated with an increase in relative orderliness for P4 and M2 at the population level. Reasoning by analogy and taking into account the relatively sedentary life style of cave bears (Ábelová 2006; Frischauf *et al.* 2015; Fortes *et al.* 2016), we can assume that different versions of the structures of P4 and M2 are fixed in different populations. Against this background, the diversity of M1 becomes more noticeable and in several cases comparable with premolar and second molar diversity.

The last tested hypothesis assumes that there is no difference between the Middle Pleistocene *U. deningeri* and the Late Pleistocene cave bears (*U. spelaeus* s. str. or *U. kanivetz* (= *ingressus*)) in terms of morphometrical diversity. This hypothesis cannot be rejected because the diversity of cheek teeth in Deninger's bear was higher than in *U. kanivetz* (= *ingressus*), at least in the final Late Pleistocene. In addition, the teeth diversity was lower in the independently evolved and more specialized Middle–Late Pleistocene Kudaro bear than in the Middle Pleistocene *U. deningeri*.

Thus, the low morphometric diversity of the upper cheek teeth in cave bears can be related to their high ecological specialization. This is especially noticeable against the background of the high diversity of cheek teeth within the brown bear lineage, which evolved for a long time in parallel with the cave bear lineage, and, owing to morphological and ecological plasticity, safely survived in the Last Maximum Glaciation, and now is amongst the flourishing Holarctic species.

## Conclusions

This paper presents the results of a new study of upper cheek teeth (P4, M1 and M2) morphometry in the cave bear evolutionary lineage (*U. deningeri*, *U. kudarensis*, *U. spelaeus* and *U. rossicus*) in comparison with its assumed Pliocene ancestor *U. minimus* and the arctoid bear lineage (*U. etruscus* and *U. arctos*). The use of multivariate analysis (NMDS multidimensional model or 'morphospace' and multivariate allometry) allowed us, in particular, to trace the evolutionary changes including progressive increase in tooth size and an allometric increase of their chewing surface, which reaches its maximum in the Late Pleistocene cave bears. Evolutionary allometry contributed to the change in shape of the molars, which manifested as the general decrease of their roundness index (IW) in the row from *U. minimus* to *U. spelaeus*. The independent evolution of P4 size and shape in the spelaeoid and arctoid lineages led to similar morphological results. The variability in M2 size and M1 shape are of great importance in differentiating amongst *U. minimus*, *U. etruscus*, *U. arctos* and

*U. deningeri*, and probably reflect the splits between them during the early stages of ursid evolution. The hypothesized evolution from *U. deningeri* to *U. spelaeus* affected the dimensions of the premolar and molars, and the shape of P4, but herewith the changes in the last tooth were of most importance. Overall, the greatest morphological disparity within cave bear taxa was in P4 sizes and, thus, variability of this tooth is potentially most useful in studying morphological differences between cave bear subspecies. The morphological classifications of the *U. spelaeus* subspecies, *U. kanivetz* (= *ingressus*) and *U. kudarensis* are in good correspondence with the schemes of their genetic differentiation based on ancient mitochondrial DNA, but the position of the small cave bear (*U. rossicus*) on the NJ tree based on the morphological data is in contradiction with the genetic data.

For the first time, in this study we used multidimensional models or 'morphospaces' not only for description of teeth size and shape variations but also for estimation of morphological diversity. Based on these models, we measured information-theoretical parameters of tooth diversity, namely, Shannon entropy and redundancy or Von Foerster orderliness. Overall, for all the ursid species studied here the first upper molar M1 shows the maximal level of orderliness of diversity in comparison with P4 or M2. Within the cave bear lineage, Deninger's bear has the greatest morphological diversity of all the teeth overall, and the lowest diversity is observed in the final taxon of this lineage – *U. kanivetz* (= *ingressus*). In the Late Pleistocene cave bear chronopopulations, the morphological diversities of P4 and M2 show multidirectional correlations with elevation above sea level, which demonstrates the sensitivity of the parameter to variation of environmental conditions. The teeth diversity was lower in the Middle–Late Pleistocene Kudaro bear (*U. kudarensis*), which evolved independently of the rest of the cave bears, and was more specialized than the Middle Pleistocene *U. deningeri*.

Finally, this study highlights the benefits of combining different multivariate and univariate statistical methods with information-theoretical parameters to improve our understanding of cheek teeth evolution within the ursid lineage and to formulate new hypotheses for further research.

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## Supporting Information

Additional Supporting Information may be found in the online version of this article at <http://www.boreas.dk>.

*Data S1.* Sexual size dimorphism of upper cheek teeth.

*Data S2.* Morphological space model. Method.

*Data S3.* Morphological diversity. Method.

*Data S4.* Supplementary data to Section ‘Morphological spaces and their interpretations.’

*Data S5.* Supplementary data to Section ‘Morphological diversity.’

*Data S6.* Supplementary data to Section ‘Multivariate allometry.’

*Data S7.* Supplementary data to Section ‘Morphometrical classifications and phylogenetic signals.’

*Table S1.* List of palaeontological sites and sample sizes.