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CONCEPTS AND METHODOLOGY TO QUANTITATIVELY RECONSTRUCT CLIMATE FROM POLLEN DATA

ABSTRACT: VALLÉ F., FURLANETTO G., MAGGI V., PINI R. & RAVAZZI C., *Concepts and methodology to quantitatively reconstruct climate from pollen data.* (IT ISSN 0391-9838, 2019).

Pollen data are widely used as *proxies* to reconstruct past vegetation and climate changes. During the last decades numerical techniques have been developed to quantitatively estimate climate parameters from fossil pollen assemblages. This contribution introduces first the concepts and methodologies based on modern calibration sets to obtain past climate reconstructions. Then, focusing on high-elevation environments, the use of elevational transects as a tool for the evaluation of pollen-climate models and a temperature reconstruction obtained from an alpine fossil site are presented. (IT ISSN 0391-9838, 2019).

KEY WORDS: Pollen data, Climate, Calibration sets, Models, Transfer functions, Reconstruction.

RIASSUNTO: VALLÉ F., FURLANETTO G., MAGGI V., PINI R. & RAVAZZI C., *Concetti e metodologia per ricostruire quantitativamente il clima da dati pollinici.* (IT ISSN 0391-9838, 2019).

I dati pollinici sono generalmente utilizzati come *proxies* per ricostruire i cambiamenti del paesaggio vegetale e del clima. Negli ultimi decenni sono state sviluppate diverse tecniche numeriche per stimare parametri climatici a partire da associazioni polliniche fossili. Questo contributo introduce dapprima i concetti e le metodologie basate su moderni datasets di calibrazione al fine di ottenere ricostruzioni climatiche del passato. Successivamente, focalizzando sugli ambienti di alta quota, vengono presentati l'utilizzo di transetti altitudinali come strumento per valutare i modelli polline-clima, e le ricostruzioni di temperatura ottenute da siti alpini fossili.

TERMINI CHIAVE: Dati pollinici, Clima, Datasets di calibrazione, Modelli, Funzioni di trasferimento, Ricostruzione.

INTRODUCTION

Climate triggers plant distribution and vegetation dynamics, due to the sensitivity of plants to air temperature, moisture ranges and soil microclimatic conditions. The widespread fossilization potential of pollen and spores (palynomorphs) in continental and oceanic sediments and the possibility of identifying them with high taxonomic resolution, promote the use of statistical methods in palynology to reconstruct past and present climate conditions. Fossil pollen records obtained from lakes, peat bogs, mires and ocean sediments are used since the early 20th century as a tool to reconstruct vegetation and environments of the past and their reaction to climate change and human pressure (e.g. Birks & Berglund, 2018).

From the qualitative description (i.e. "colder", "warmer", "wetter", "temperate") of past Quaternary climates inferred from microfossil assemblages, a step further towards quantitative reconstruction of environmental and climate parameters has been done during the last 50 years. Different procedures were developed to quantitatively estimate past temperature, precipitation, bioclimatic indexes, chemical and trophic state of water bodies from stratigraphical microfossil assemblages (chironomids: Eggermont & Heiri, 2011; chrysophytes: Kamenik & Schmidt, 2005; cladocera: Brodersen & *alii*, 1998; diatoms: Birks & *alii*, 1990) including pollen data (e.g. Birks 1995, Birks, 2003, Seppä & *alii*, 2004 and reference therein, Brewer & *alii*, 2007, Kamenik & *alii*, 2009, Juggins & Birks, 2012). Thus, quantitative reconstructions from biological proxies using the so-called "transfer functions" have revolutionised palaeolimnology (Juggins, 2013).

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The potential of pollen assemblages as direct quantitative descriptors of past climate conditions is gaining increasing interest in the Quaternary community (Juggins & Birks, 2012); therefore it is necessary to directly link modern climate and modern pollen data in order to apply those relationships back in the past. Pollen stratigraphical researches can indeed be coupled with quantitative climate reconstructions based on the same compilation of data thus providing new hints for the interpretation of palaeoecological records and also improve our understanding of man-environment interactions. Furthermore, quantitative climate reconstructions from microfossil assemblages are useful for both multi-proxy reconstructions and for validation of the results of global circulation and climate models (Brewer & *alii*, 2007), especially for pre-instrumental periods and much older intervals (e.g. Fauquette & *alii*, 1998; Bartlein & *alii*, 2011 and references therein).

This work will first focus on principles, requirements and numerical techniques to obtain quantitative climate reconstructions from pollen data, discussing also strength and weaknesses. Afterwards, we present case studies of reconstructions for different time intervals in northern Italy and their evaluation using instrumental data and other climate proxies.

BASIC PRINCIPLES AND ASSUMPTIONS FOR CLIMATE RECONSTRUCTIONS FROM POLLEN DATA

The basic principle of quantitative climate reconstructions from biological data is the "methodological uniformitarianism" (Birks & Birks, 1980, Birks & Seppä, 2004, Brewer & *alii*, 2007, Birks & *alii*, 2010 and references therein): as far as palynological data are concerned, the relationships between modern pollen-climate data can be used as analogue or model to infer past conditions assuming that those relationships have not changed throughout time. In fig. 1 the uniformitarianism principle and its major requirements are outlined, namely, the existence of a modern calibration (or training) set composed by modern pollen assemblages and associated climate variables.

At least six assumptions at the base of quantitative climate reconstructions from biological assemblages were defined by Birks & *alii* (2010) (and reference therein) and Telford & Birks (2009) and hereafter recalled:

1) The taxa in the modern calibration set are systematically related to the environment in which they live;

2) the climate variable(s) to be reconstructed is, or is linearly related to, an ecologically important determinant in the system of interest;

3) the taxa in the calibration set are the same biological entities as in the fossil data and their ecological responses to the climate variable(s) of interest have not changed over the time represented by the fossil assemblage;

4) the numerical methods adequately model the biological responses to the climate variable(s) of interest and yield numerical models that allow accurate and unbiased reconstructions;

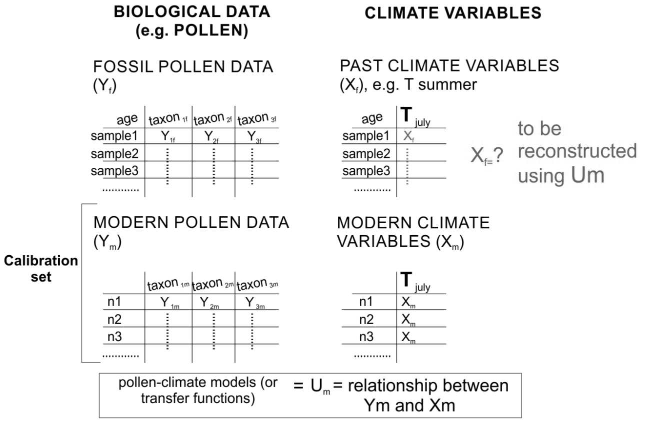

FIG. 1 - Scheme of the basic principles for quantitative climate reconstructions from pollen data. Y are pollen taxon abundances (percentages), X are climate variables. Xf, the unknown climatic variable to be reconstructed from fossil pollen assemblages Yf, the essential role of a modern calibration set consisting of n= modern pollen assemblages and associated climate values, and the resulting transfer function (Um) (modified from Birks & Seppä, 2004; Birks & *alii*, 2010).

5) climate variables other than the one to be reconstructed have negligible influence, or their joint distribution with the climate variable does not change with time;

6) during the model validation process, the test data are statistically independent from the calibration set in use.

Generally, the transfer functions or pollen-calibration models (Um) are the ecological functions "*f*" necessary to solve the equation $Ym = f(Xm) + error$ (Juggins & Birks, 2012). The summarized methodology to obtain quantitative climate reconstructions from biological data involves "three steps" (Juggins & Birks, 2012): 1) the development of a calibration set representative for the variable to be reconstructed, 2) the application of numerical methods to the modern pollen-climate data to model their relationships (or finding the transfer function), and 3) the application of the best model (or transfer function) to the stratigraphical-pollen records to finally estimate the past climate values, the validation of the models developed and the obtained reconstruction. Concepts and steps procedure are presented in the flow diagram below (fig. 2). Each of the steps and requirements will be discussed in detail in the next sections.

MATERIALS AND METHODS TO DEVELOP POLLEN-CLIMATE MODELS AND TRANSFER FUNCTIONS

Modern calibration sets (pollen data and related climate variables)

The base for modelling pollen-climate relationships is the calibration dataset composed by modern pollen assemblages and associated measured climate variables. The development of a new calibration set or the selection of an existing one must be adequate to the environmental context from which the fossil pollen record is obtained, and the goodness of the climate reconstructions depends mostly on the ecological and climate structures and distribution

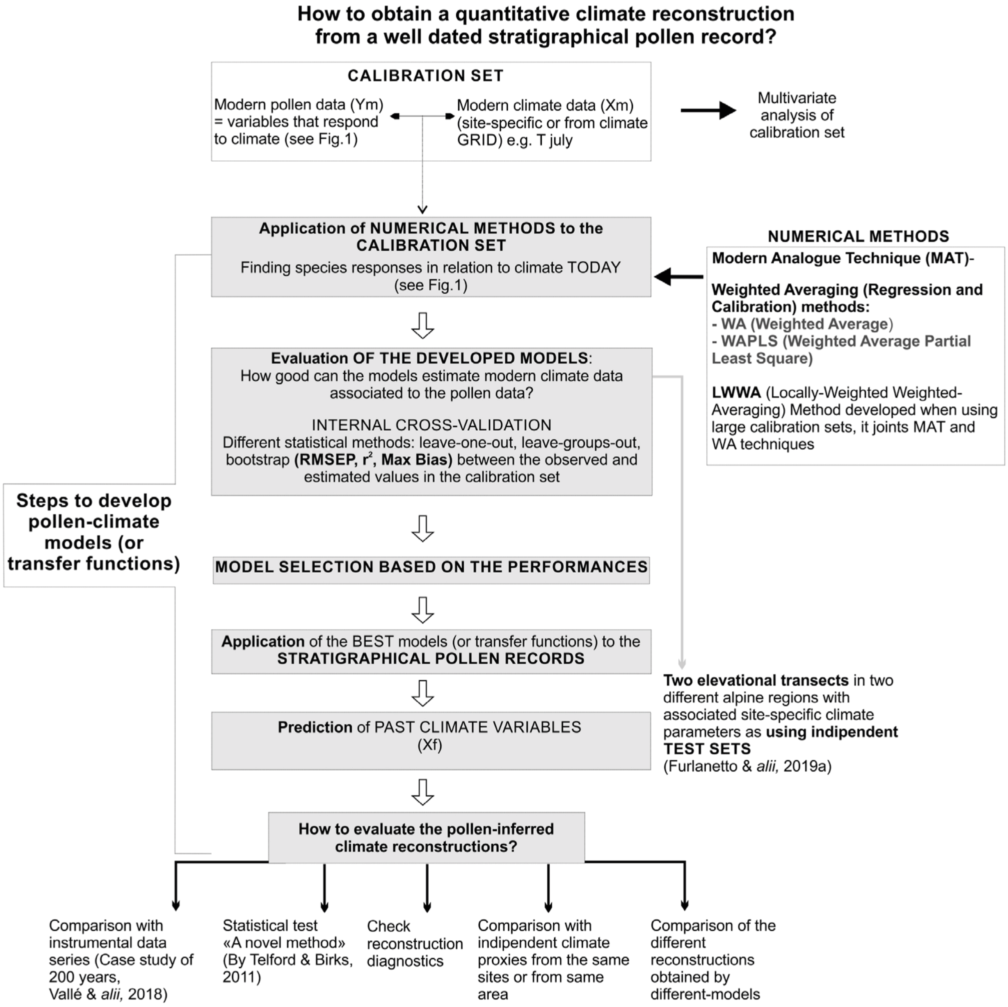

FIG. 2 - Flow diagram showing the procedure used to obtain and validate quantitative past climate reconstructions from pollen data.

of the modern calibration set. A calibration set is arranged in two matrices (fig. 1). The first matrix includes the modern pollen assemblages which indeed represent samples of the modern pollen deposition possibly occurring in different sedimentary environments. The concepts of pollen dispersal, transport and deposition in diverse depositional settings are illustrated in fig. 3A. Since most of the fossil pollen records allowing a continuous registration of past environmental and climate changes in northern Italy are from lakes or mires, a focus on the ways to sample the modern pollen deposition in those environmental contexts is summarized in fig. 3B.

Each pollen taxon identified in a modern pollen assemblage is commonly expressed by pollen percentages. During the last years, different pollen-climate databases at continental or regional scales became available thanks to the contribution of several analysts. As far as Europe is concerned, the European Modern Pollen Database (EMPD; Davis & *alii*, 2013) consists of more than 4200 modern pollen samples from Eurasia (fig. 4). Climate data associated to each of the EMPD modern pollen sample are generally computed from the WorldClim, global GRID climatology of Hijmans & *alii* (2005). The EMPD modern pollen assemblages were sampled by using several types of natural pollen traps (fig. 3B), while artificial pollen traps were excluded because of their short time recording (Davis & *alii*, 2013). This continental scale dataset is used as source for statistically based comparisons between fossil and modern pollen spectra. Although the relevance of this dataset is undeniable, several points need to be fixed in order to provide the Eurasian pollen-community with an ecologically sound and complete tool for palaeoclimate reconstructions.

Analysis of the calibration set and relationship with climate parameters

A first analysis of the calibration sets is necessary to check whether a parameter may be subjected to reconstruction, avoiding to and explicitly address the dangers of reconstructing surrogate and confounded variables (Juggins, 2013). The variable of interest needs to explain a relevant portion of the variability of modern pollen assemblages included in the calibration set. Multivariate analyses of the calibration sets, both unconstrained (e.g. Detrended Correspondence Analysis, DCA) and constrained (e.g. Canonical Correspondence Analysis, CCA) help exploring

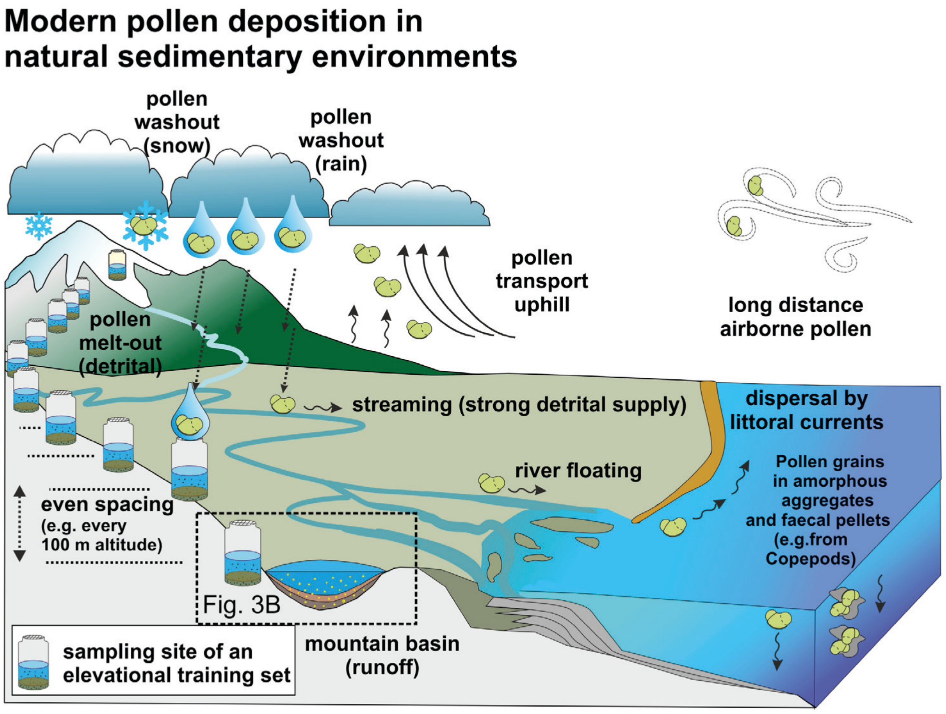

FIG. 3A - Pollen dispersal across a mountain region facing a sea basin, and deposition in natural sedimentary environments. Pollen grains, especially those produced by anemophilous plants, are first dispersed in the air masses, washed out by rain and snow, deposited on the ground, water and glaciers surfaces. Grains melted out from glaciers as detrital particles, streamed along water courses or by slope runoff, can be also decanted in water columns or trapped by organisms, and finally, deposited. Pollen wall, made of sporopollenin, allows for effective preservation in soils and in sediment layers at the bottoms of ponds, mires, lakes, or oceans. On the left side of the figure, the sampling strategy developed in mountain environments is sketched. Additionally, through the ocean water column pollen grains might be agglomerated in faecal pellets or amorphous aggregates and rapidly sink into the ocean floors (Hooghiemstra & *alii*, 2006).

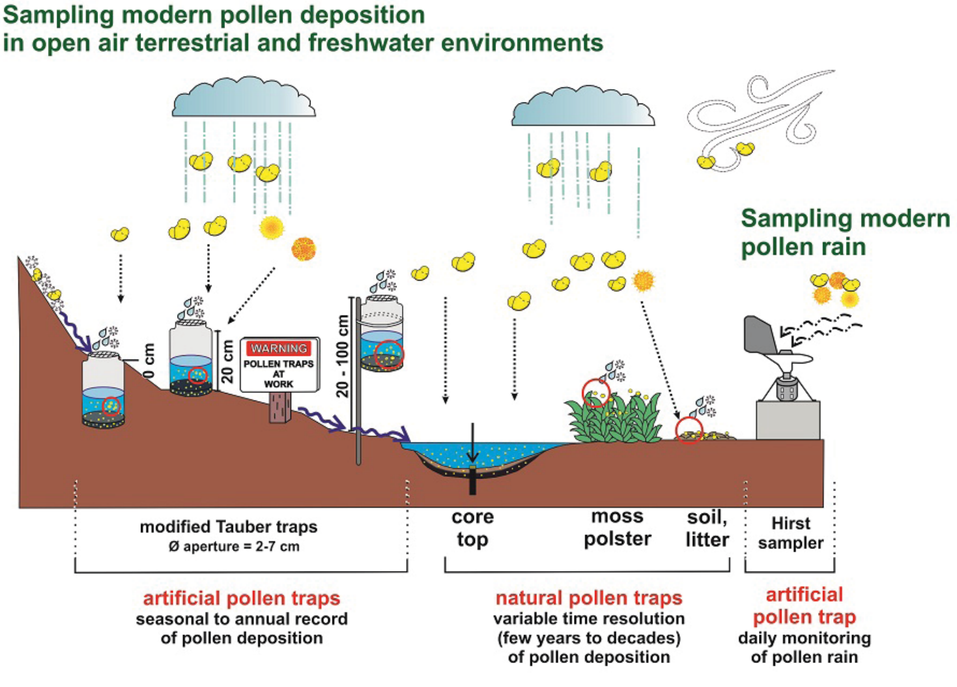

FIG. 3B - Sketch illustrating strategies to sample pollen and other airborne particles in the atmospheric boundary layer (pollen rain) and in open air terrestrial and freshwater environments, such as ground surfaces in small basins depositional environments (pollen deposition). The strategies are adapted to mountain or subalpine areas, where runoff and snow runoff are very important vehicles affecting particle dispersal and deposition. Snow runoff and slope runoffs are presented with dark blue wavy arrows. At the right edge of the figure, the Hirst sampler is sketched: this tool allows for a direct sampling and monitoring of the atmospheric boundary layer at a given height above ground level.

the ecological and climate gradients lengths and the relationships between pollen taxa and climate variables. Recent exploratory work on pollen-climate calibration sets highlighted that July mean temperature (Tjuly) (see tab. 1) and summer precipitation explain a significant portion of the variance in the modern pollen assemblages of the Alpine region (Finsinger & *alii*, 2007), while these parameters do not work in the Mediterranean ecosystems affected by strong drought gradients.

Numerical methods to develop pollen-climate models (or transfer functions)

Several numerical techniques have been developed, given that each method has its strength and weaknesses (Birks & *alii*, 2010). All numerical methods can be explored using the R software (R Core Team, 2017) and available R packages (e.g. Rioja Package, Juggins, 2017).

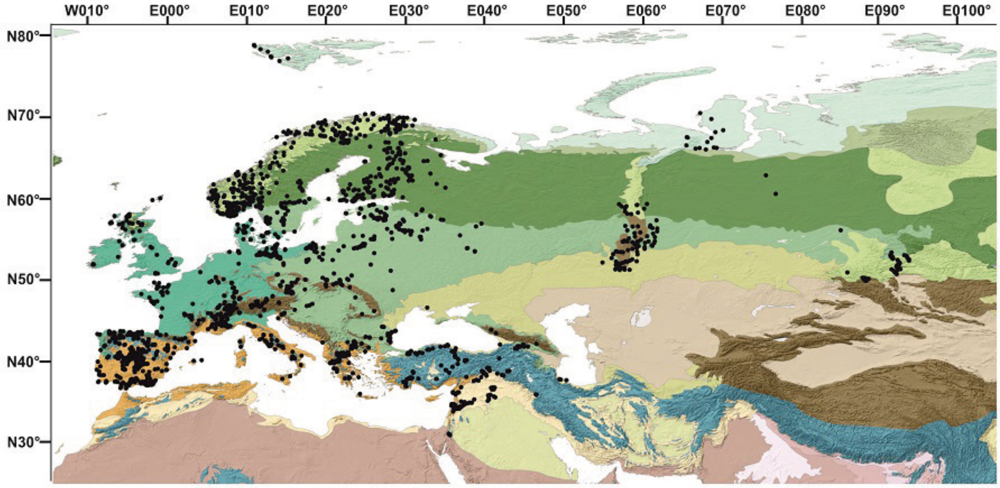

FIG. 4 - Geographical extent of the European Modern Pollen Database (EMPD: Davis & *alii*, 2013) excluding north African samples. Black dots indicate the location of the 4270 sampling sites superimposed on the spatial distribution of global ecological zones (GEZ) proposed by the Global Forest Resources Assessments (GRFA) of FAO (http://www.fao.org/forest-resources assessment/remote-sensing/global-ecological-zonesgez/en/). Pollen and climate data and metadata associated to each EMPD site shown in the map can be downloaded at http://www.europeanpollendatabase.net/wiki/doku.php?id=empd_download_database.

Method based on similarity: the Modern Analogue Technique (MAT)

The Modern Analogue Technique (MAT) (e.g. Guiot, 1990; Juggins & Birks, 2012) is based on the similarity between fossil pollen assemblages and modern pollen samples (or analogues) available in the calibration set. The resemblance is evaluated based on squared-chord distances, measured after square-root transformation of pollen percentages to reduce the influence of few relatively abundant taxa occurring in the samples (Brewer & *alii*, 2007). Once the modern analogues have been selected, climatic values can be attributed to the fossil sample as a weighted average of the climate of the modern samples. The weights used are the inverse of the chord distance, which allows the most similar analogues to have the greater influence on the climate estimates obtained. The number of analogues is chosen during the process of internal cross-validation. MAT diagnostics allow the recognition of the possible "no-analogue" situations (Juggins & Birks, 2012).

Methods based on taxon-climate response models: Weighted Averaging (WA) and Weighted Average - Partial Least Squares (WA-PLS)

The methods based on the taxa response models to the climate variables can be described as a regression-calibration procedure. They imply that species occupy different niches in climate space, and that these niches can be characterized by parameters describing the niche centre (optima) and niche breadth (tolerance) (e.g. Juggins & Birks, 2012, Birks & *alii*, 2010 and references therein). The ecological response function is the unimodal relationship in which taxon abundance varies across the environmental gradient, with an optimum at a particular value. The weighted averaging technique (WA; ter Braak & Barendregt, 1986) allows these unimodal response functions to be used in climatic reconstructions (Juggins & Birks, 2012 and references therein, Brewer & *alii*, 2007). The regression step of WA consists of estimating the optima of the selected taxa for a given climatic or environmental parameter by weighted-averaging the climate values over the modern assemblages where the species is found (Birks & *alii*, 2010, Juggins & Birks, 2012); this procedure is repeated for all taxa present in the fossil sample (Brewer & *alii*, 2007).

WA-PLS method combines WA and partial least square (ter Braak & Juggins, 1993) and tries to solve the "edge effect" affecting WA by using residuals correlations. The WA-PLS method considers different components (up to 5) of the whole taxa in the calibration set, calculated as weighted average of the taxa scores in the regression step.

Locally-weighted weighted-average (LWWA)

When the fossil pollen record extends over a long-time interval under different climate conditions and when calibration sets cover long ecological/climate gradients, the LWWA method, combining the MAT and WA methodologies, can be used. WA method is applied to the selected analogues (Juggins & Birks, 2012 and references therein).

TABLE 1 - Results of canonical correspondence analysis (CCA) applied to the modern pollen assemblages distributed along elevational transects in La Thuile Valley and Upper Brembana Valley (modified from Furlanetto & *alii*, 2019a). The mean temperature of the warmest month (July, CCA axis 1) explains significantly (p-value = 0.001) in both Valleys the variability of the pollen dataset. The percentage of variance explained in the La Thuile Valley elevational transect is 12.3% and the ratios between the constrained axis and the first unconstrained axis (λ1/λ2) is close to 1. In the Upper Brembana Valley the percentage explained is lower because secondary gradients (e.g. different aspect) influence the variability in pollen assemblages.

	Tjuly		
La Thuile Valley	CCA1	CA 1	λ1/λ2
Eigenvalue	0.09601	0.1072	0.9
Percentage variance (%)	12.3	13.7	
P-value	0.001***		
Upper Brembana Valley	CCA1	CA 1	λ1/λ2
Eigenvalue	0.07313	0.1207	0.6
Percentage variance (%)	8.23	13.6	
P-value	0.001***		

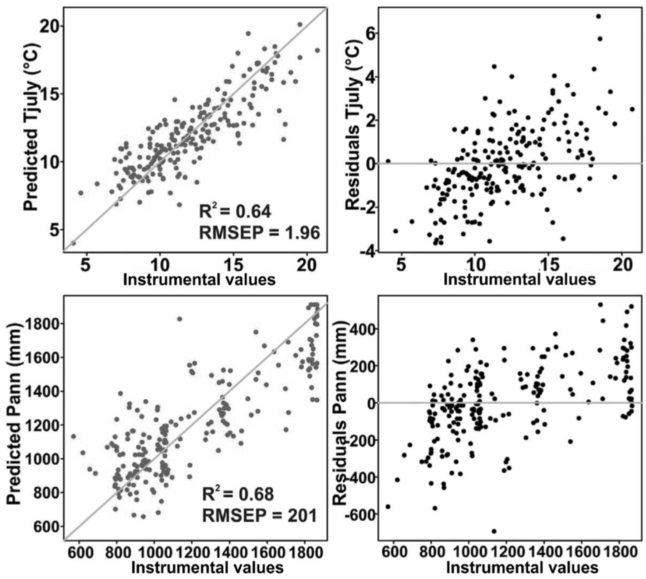

FIG. 5 - Cross-validation results for the pollen-climate models developed to reconstruct Tjuly and Pann at Armentarga fossil pollen record, Central Italian Alps. Instrumental data Tjuly (°C) and Pann (mm) are plotted against pollen-inferred values (WA-PLS model) (left side) and residuals against the instrumental values (right side) obtained from the cross-validation of the WA-PLS model developed calibration set (modified from Furlanetto & *alii*, 2018).

Evaluation of models and reconstructions developed

Pollen-climate models (or transfer functions) developed with the numerical methods listed above are submitted to validation. Model performances were obtained using internal cross-validation within the calibration set. This procedure allows the assessment of the model errors in estimating the observed values. The parameters to be considered from the cross-validation are the root mean square of predictions, the r between observed and estimate values and the residual plots. Examples of cross-validation results are shown in fig. 5. Models evaluation is necessary for MAT in order to choose the number of analogues to be selected and for WA-PLS in order to determine the number of components to be used in the final step, i.e. the application of the models to the fossil pollen record.

A good model performance does not assure alone, that the past climate reconstructions obtained applying the models developed to the fossil pollen records are reliable (e.g. Juggins & Birks, 2012). Thus, the finally obtained past climate reconstructions need also evaluation (see fig. 2). The evaluation of past climate reconstructions obtained from palynological data for intervals older than the instrumental data are only possible using statistical tests and procedures (e.g. Juggins & Birks, 2012 and references therein) or by comparison with other climate proxy from the same study site or from the regional area.

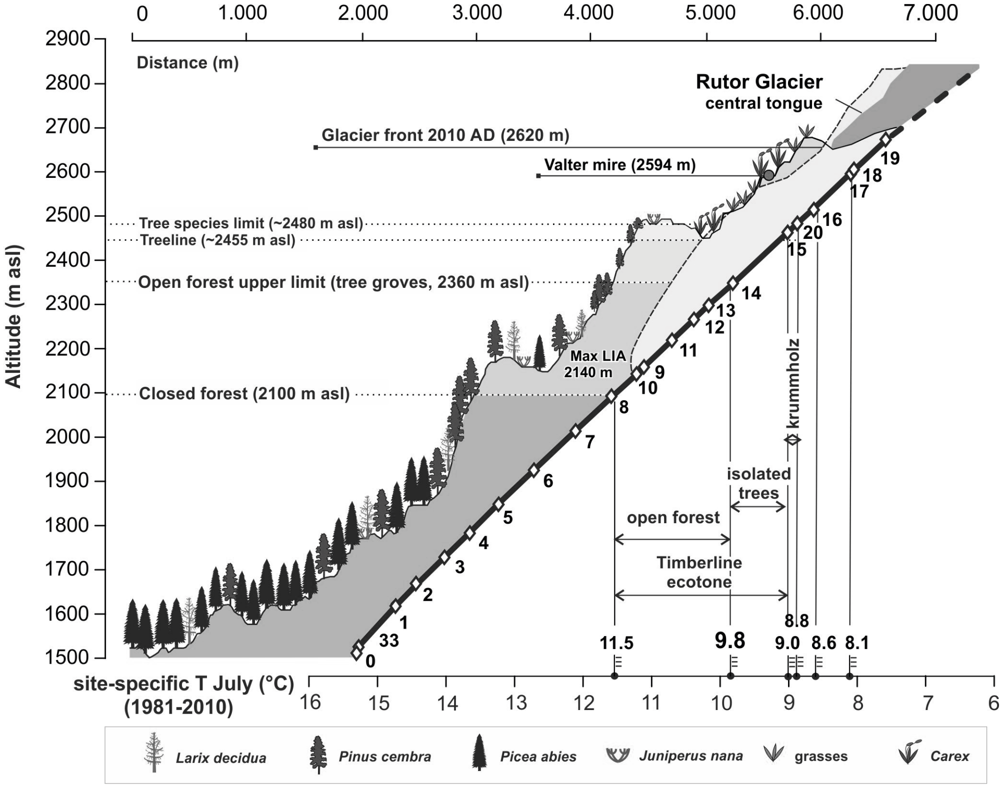

FIG. 6 - Sketch of the elevational transect developed in La Thuile Valley from 1500 to 2700 m aslat the front of the Rutor Glacier. Present-day vegetation types and modern T july values associated (computed from M. Brunetti, ISAC-CNR) to elevational limits are shown (modified from Badino & *alii*, 2018).

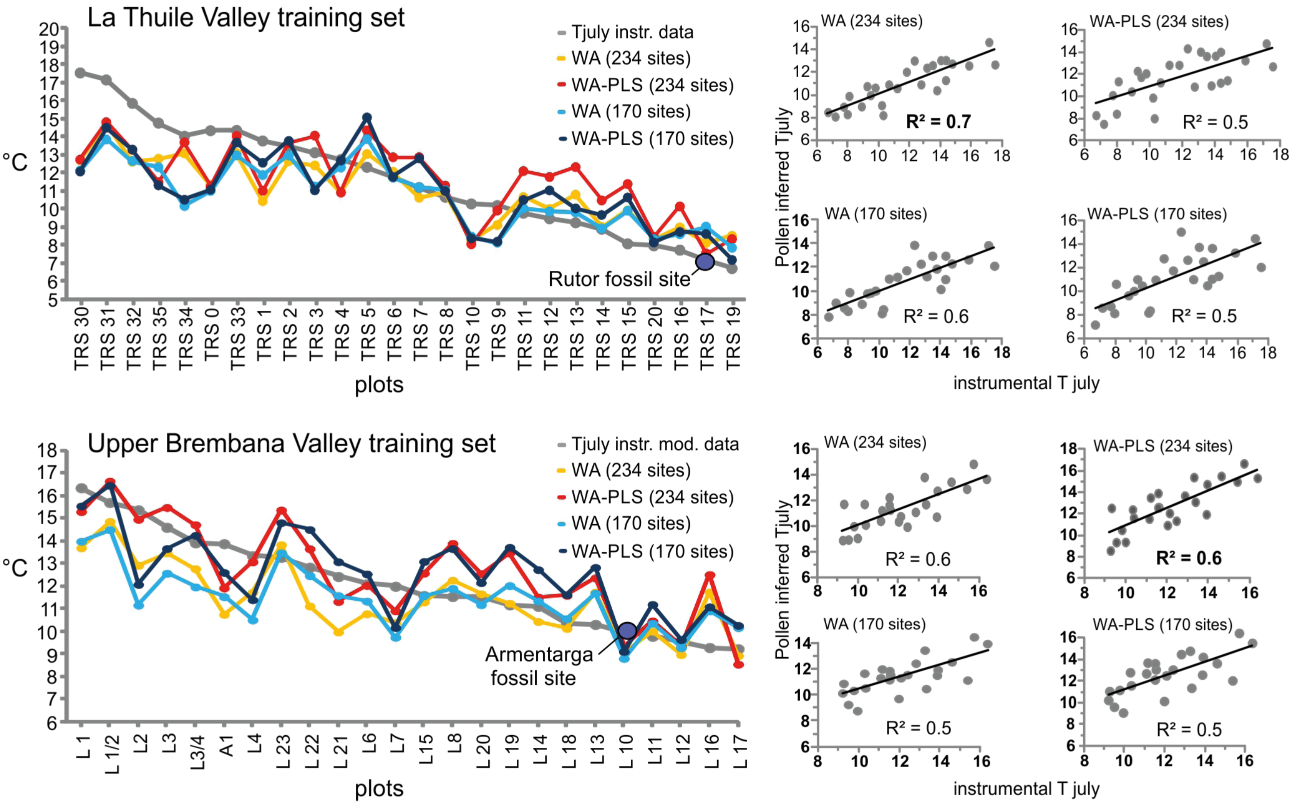

FIG. 7 - Comparison and correlation between pollen-inferred Tjuly obtained along the two elevational training sets developed in La Thuile Valley and Upper Brembana Valley and the instrumental values computed for each plot of the training sets. Pollen-climate models (WA and WA-PLS) have been developed using two calibration sets selected from the European Modern Pollen Database (EMPD, Davis & *alii*, 2013). (modified from Furlanetto & *alii*, 2019a).

TEST SETS FOR THE EVALUATION OF POLLEN-CLIMATE MODELS IN THE ALPS

Two calibration sets of modern pollen rain - vegetation cover - climate data - terrain parameters were developed in the western and central Alps (La Thuile and Brembana Valleys, respectively Badino, 2016; Furlanetto & *alii*, 2019a; Furlanetto & *alii*, 2019b) to support reconstructions from high-elevation fossil records developed in the same areas. The aim of such big efforts was to obtain valley-specific proxies' calibration along elevational transects and to improve our knowledge on the relationships between the selected parameters. At each sampling site vegetation surveys and monitoring of modern pollen deposition through the analysis of moss samples were carried out: moreover, site-specific temperature and precipitation series, covering the 1951-2015 period, were computed by means of the anomaly method (New & *alii*, 2000; Mitchell & Jones, 2005) as described in Brunetti & *alii* (2006, 2012, 2014). An example of elevational training set is shown in fig. 6 (modified from Badino & *alii*, 2018). The modern vegetation types distribution has been associated to its modern climate values. Data collected with our two alpine calibration sets were used, along with the EMPD data, for temperature and precipitation reconstructions based on high-altitude Holocene pollen records obtained in the continental western Alps (Badino & *alii*, 2018) and in the external alpine chains of Lombardy affected by oceanic climates (Furlanetto & *alii*, 2018). Both elevational transects were used as independent test sets to validate pollen-climate models developed for high-elevation sites using calibration sets selected from the European Modern Pollen Database (Davis & *alii*, 2013). Transfer functions obtained with these calibration sets were applied to the transect samples, for which instrumental climate data were available (fig. 7). The differences between observed and estimated climate values at the different elevational locations provide hints to better understand issues related to past climate reconstructions (Furlanetto & *alii*, 2018, 2019a).

EXAMPLE OF HOLOCENE TEMPERATURE RECONSTRUCTIONS FROM HIGH ELEVATION SITE IN THE WESTERN ALPS AND COMPARISON WITH OTHER CLIMATE PROXIES

A reconstruction of July temperature (Tjuly) going back to 8800 years cal BP has been obtained for a high-altitude area in the western Alps, at the front of the Rutor Glacier (fig. 8, modified from Badino & *alii*, 2018). This reconstruction was obtained with a MAT model based on 5 analogues. Trends and variations observed in the reconstructed temperature record were evaluated by means of the statistical test suggested by Telford and Birks, 2011 (see Badino & *alii*,

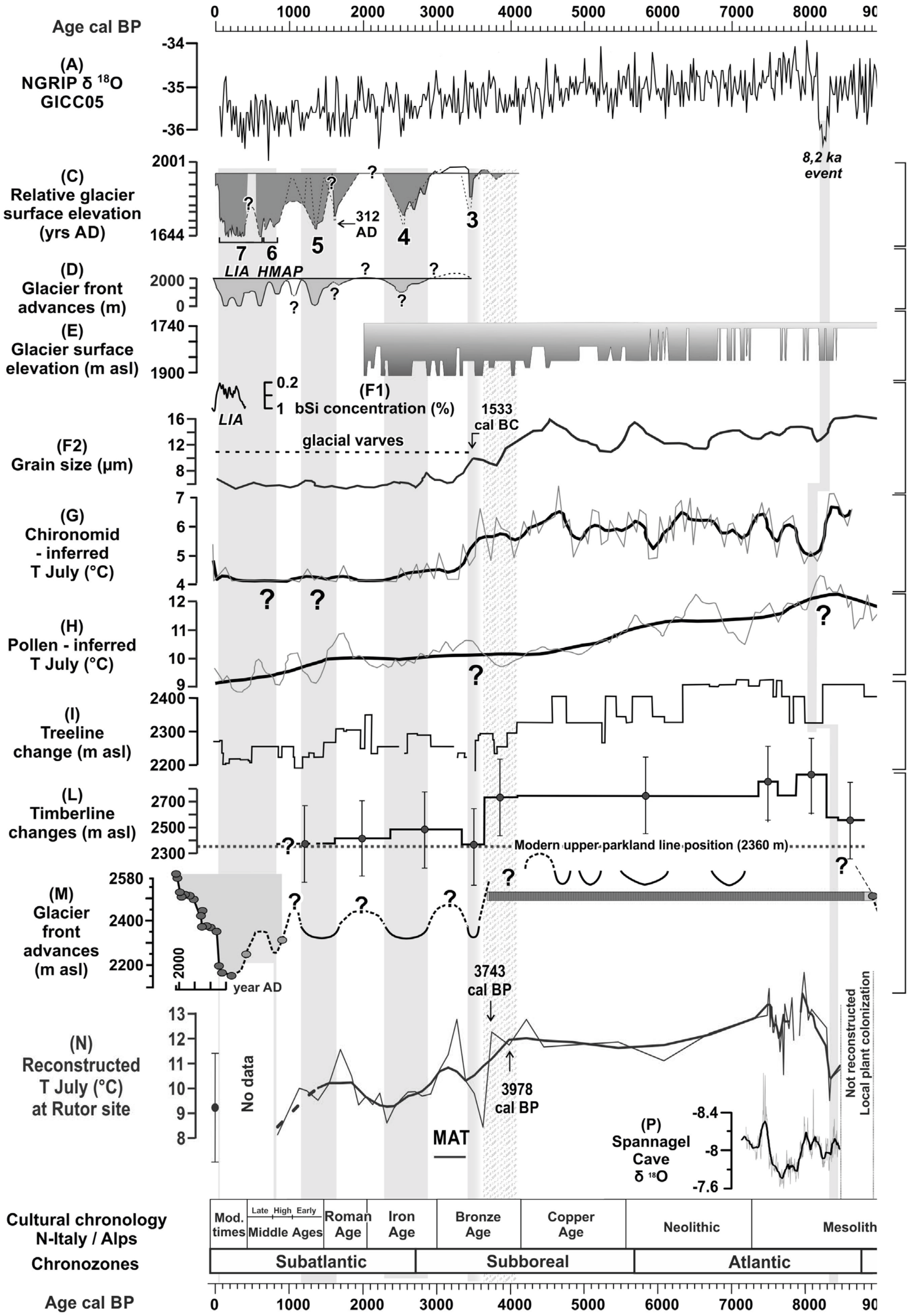

FIG. 8 - Tjuly (panel N) reconstructed from a fossil peat archive in the high-altitude Rutor Glacier forefield area (La Thuile Valley, western Italian Alps) is compared with other climate proxy records from the Alpine region and the global isotope record of the NGRIP (modified from Badino & *alii*, 2018; see references therein). Thin black line represents the reconstruction while thick black line is the smoothed reconstruction.

2018) and by comparison with other independent climate proxies (fig. 8). The major cold event at 8.2 ka recognized at global scale in the NGRIP isotope record (A, in fig. 8) is also visible in the Rutor July temperature record.

CONCLUSIVE REMARKS

We have presented the most used methodology, based on the use of modern pollen-climate calibration datasets and the developed transfer functions, to obtain quantitative climate reconstructions.

We discussed two case studies from the Alpine region as examples of the application of this methodology, highlighting the validation technique and some of the weaknesses of the considered numerical methods, especially when focusing on mountain environments, that are poorly considered as region where quantitative methods can be applied.

The multivariate complexity of the relationships between biological data and their physical environments or climate accounts for part of the problems of the reconstruction methods (Juggins, 2013). Improvements of the existing numerical methods and the developments of other reconstruction techniques based on Bayesian approach, independent from the existing relationships between pollen and climate, will enhance the use of pollen data as direct climate proxy.

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