EFFICIENT RECONSTRUCTIONS OF COMMON ERA CLIMATE VIA INTEGRATED NESTED LAPLACE APPROXIMATIONS.

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ABSTRACT. A Paleoclimate Reconstruction on the Common Era (1-2000AD) was performed using a Hierarchical Bayesian Model from three types of data: proxy data from PAGES2k project dataset, HadCRUT4 temperature data from the Climatic Research Unit at the University of East Anglia, and external forcing data from several sources. Five data reduction techniques were explored with the purpose of achieving a parsimoneous but sufficient set of proxy equations. Instead of using the MCMC approach to solve for the latent variable, we employed an INLA algorithm that can approximate the MCMC results and meantime is much more computationally efficient than MCMC. The role of external forcings was investigated by replacing or combining them with a fixed number of BSplines in the latent equation. Two different validation exercises confirm that it is feasible to improve the predictive ability of traditional external forcing models.

1. INTRODUCTION.

Earth’s climate presents a continuum of variability, with periodic and non-periodic fluctuations ranging from 1 to $10^8$ years [Pelletier, 1998; Ghil, 2002; Huybers and Curry, 2006]. In particular, variability on scales of decades to centuries is of paramount importance for adaption and planning to anthropogenic climate change, yet is incompletely sampled by the relatively short historical record of wide-spread instrumental observations, going back to about 1850 CE [Masson-Delmotte et al., 2013]. It is thus critical to reconstruct these variations from the paleoclimate record as quantitatively as possible. A particular focus has been reconstructions of global or hemispheric temperature from high-resolution proxy observations [Jones et al., 2009].

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Many methods have been developed to reconstruct past climates, particularly temperatures: principal component regression (Mann et al., 1998, 1999; Luterbacher et al., 2004; Wahl and Smerdon, 2012; Neukom et al., 2014), regularized forms of the expectation-maximization algorithm (Schneider, 2001; Rutherford et al., 2005; Mann et al., 2005, 2007; Rutherford et al., 2003; Steig et al., 2009; Emile-Geay et al., 2013a,b; Guillot et al., 2015), canonical correlation analysis (Smerdon et al., 2010; Wang et al., 2014; Evans et al., 2014), pairwise comparison (Hanhijärvi et al., 2013; Gergis et al., 2016), data assimilation (Lee et al., 2008; Hakim et al., 2016), and Bayesian hierarchical models (BHM).

BHM offer several distinct advantages for paleoclimatic reconstruction. They can (i) treat different sources of uncertainty in a natural way (ii) incorporate prior knowledge of the system in a logically-coherent manner (Jaynes, 2004) (iii) allow for both inference and prediction (Tingley et al., 2012). Many studies have conducted BHM: Li et al. (2010); Tingley and Huybers (2010a,b, 2013); Werner et al. (2013); Barboza et al. (2014) are examples among others. Some of these studies have used space-state schemes to linearly relate information that comes from paleoclimate observations (coming from trees, corals, icea cores, lake and marine sediments, and historical archives) together with information about external climatic forcings, resulting from well-mixed greenhouse gases, volcanic activity, and variations in solar output. Three problems arise in this case: the need to reduce dimensionality, the complexity/realism of the model, and the execution time of the numerical procedure.

Barboza et al. (2014) proposed a method that jointly models the variability of the temperature series (as a latent process) as well as the variability of those climatic and biological variables that serve as approximations of this process. The authors found that long memory error terms are necessary in absence of external forcing information within a BHM, but the presence of external forcing information substantially improves the reconstruction. The scope of the study was restricted by the computational requirements of the Monte Carlo Markov Chain (MCMC) procedure, which limited the sensitivity analysis and forced severe levels of data reduction.
In this article we leverage Integrated Nested Laplace Approximations (INLA) to extend the work of Barboza et al. (2014). By lightening the computational burden, INLA allows to (a) explore new model designs inspired by the physics of the problem; (b) consider various choices for data reduction; and (c) take the non-stationary nature of the observational network into account. In addition, this work makes use of the most up-to-date estimates of radiative forcing, as well as a state-of-the-art, open-access compilation of community-curated paleoclimate observations (Emile-Geay et al., 2017). This ensures that our calculations are using the best available data and are completely reproducible.

The article is organized as follows: we start by describing the datasets (section 2), and the methodology (section 3). Results are presented in section 4, discussed in Section 5, before concluding in section 6.

2. Datasets.

2.1. Proxy data. Reconstructions of past climates rely on “proxies”: indirect observations of climate, as recorded in borehole, coral, documentary, glacier ice, lake and marine sediment, sclerosponge, speleothem and tree-ring archives (Jones et al., 2009).

The PAGES2k global multiproxy database is a “community-driven effort to synthesize all publicly-archived, temperature-sensitive proxy records of the past 2,000 years” (PAGES2K Consortium, 2013; Kaufman, 2014; Emile-Geay et al., 2017). The most recent effort (Emile-Geay et al., 2017) made all records available in a standard format (LiPD, McKay and Emile-Geay, 2016) readable in R, Python and Matlab (McKay et al., 2016), to ensure reproducible workflows.

The dataset gathers collected through 692 data series from 648 locales around the world. Each of those proxies has different time horizons (Fig. 1.1 bottom), which creates challenges for inference. Unlike previous studies (for example Barboza et al. (2014)), we strive to take into account the information available in most proxies, despite their temporal diversity. In order to select proxies with high predictive power, we first chose those series with large correlations with respect to their closest spatial temperature record in the HadCRUT4.2
dataset (Morice et al., 2012). More details on this “screening” procedure, which controls for the multiple test problem (Benjamini and Hochberg, 1995), can be found in (Emile-Geay et al., 2017); it whittles down the database to 257 proxies (Fig. 1).

2.2. Temperature data. We estimate Global Mean Surface Temperature (GMST) from the HadCRUT4 global temperature dataset provided by the Met Office Hadley Centre and the Climatic Research Unit at the University of East Anglia, UK (version 4.4.0.0). The dataset consists of instrumental, in situ observations of surface temperature over land (Jones et al., 2012) and ocean (Kennedy et al., 2011b,a). The observations are expressed as anomalies relative to the monthly-mean seasonal cycle over the 1961-1990 period, in degrees Celsius. Though HadCRUT4 features a rather sophisticated analysis of error sources (Morice et al., 2012), as a 100-member ensemble of draws from the error distribution, we neglect these uncertainties against the much larger uncertainties affecting paleoclimate observations, and simply use the median of this ensemble, averaged on an annual basis.

2.3. Forcing data. It is well-known that climate responds to external forcings, including natural forcings. In this work we take advantage of this knowledge for statistical modeling,
and use the most recent compilations from the PMIP4-CMIP6 project (Jungclaus et al., 2017; Kageyama et al., 2017). The data consist of:

- Volcanic forcing from the Easy Volcanic Aerosol (EVA) dataset (evolv2k, Toohey et al. (2016)), which reconstructed zonal mean AOD (mid-visible, i.e., 550 nm), covering the 500 BCE to 1900 CE time period. For 1900 (or 1850) to present, Thomason et al. (2016) is used to fill in the forcing table. EVA is given as a function latitude, so the data are area-weighted (multiplied by the cosine of their corresponding latitudes) and averaged to form a global estimate (Fig. 2, top).

- The solar forcing data is computed from the SATIRE-H (Holocene) dataset (Vieira et al., 2011). Irradiance from SATIRE-H (Holocene) is provided on a decadal basis from 9495BC - 1939AD and then on a daily basis from 1940AD onwards. Hence, the data prior to 1939AD was interpolated using splines and after 1940AD, at annual resolution. For consistency, daily data from 1640AD to 2000AD is also spline interpolated to annual resolution (Fig. 2, middle).

- Greenhouse-Gases concentrations: hemispheric means of mole fraction of carbon dioxide in air (ppm) with annual resolution (Meinshausen et al., 2017) as well as ice core measurements prior to that date (Jungclaus et al., 2017) (Fig. 2, bottom).

3. Methodology

3.1. Data reduction methods. The proxy data matrix is large ($p = 257$) compared to the 101 yearly samples used to train the model (1900-2000). This large $p$, small $n$ problem therefore require a data reduction of some kind. Following Barboza et al. (2014), we do so by generating a set of “Reduced Proxy” ($RP$) time series, which condense individual proxy time series into a single time series with larger predictive power over the GMST target. Since this is one of the major steps in temperature reconstruction, in this paper we will carefully investigate five common data reduction methods rather than adopting the simple data reduction method employed in Barboza et al. (2014), after some initial screening of proxies series.
Figure 2. Main climate forcings of the Common Era (1-2000 AD): volcanic, solar, and carbon dioxide. AOD = Aerosol optical depth. TSI = total solar irradiance. ppm = parts per million. See text for details.

| Group | Interval (year AD) | Number of Proxies |
|-------|--------------------|-------------------|
| 1     | 1-250              | 19                |
| 2     | 251-500            | 25                |
| 3     | 501-750            | 29                |
| 4     | 751-1000           | 33                |
| 5     | 1001-1250          | 54                |
| 6     | 1251-1500          | 65                |
| 7     | 1501-1750          | 105               |
| 8     | 1751-2000          | 146               |

Table 1. Distribution of proxies according to their temporal availability.

The 257 proxy variables are first centered and scaled. Then we remove proxy series whose proportion of missing annual observations is larger than 5% during the calibration period. Due to the diversity of start dates in the proxies database (Fig. 1), we gather proxies into non-homogeneous groups where each group has temporal availability within a 250y interval. As the reconstruction is taking place over a 2000 year horizon, this creates 8 groups with the distribution shown in Table 1.
An important aspect we notice from the distribution of Table 1 is that the number of proxies can be greater or close to the number of available observations in the calibration period defined as 1900-2000CE (101 observations), which can cause overfitting issues or dimensionality problems with classical linear models. The choice of the calibration period is based on the arguments shown in Barboza et al. (2014). For the above reasons, we investigated various data reduction techniques with the aim of establishing a reliable linear model between the observed anomalies and the corresponding proxies in Table 1 based on the data in the calibration period. Many different data reduction methods have been developed; we focus on five popular ones:

**Lasso Regression (LR):** The Lasso regression penalizes the usual sum of squares with an argument containing the sum of the absolute values of each coefficient in the classical linear regression model, multiplied by an additional smoothing parameter (Tibshirani 1996). Due to the geometric nature of the term of penalization, the search of estimators tends to assign values very close to zero to variables that have almost null effects with respect to the dependent variable, which makes the resulting models easily interpretable. This method is very common to data reduction and easy to implement, but it often tends to select models with an excess of complexity, that is, it tends to show "false positives" in the variable selection process (Fan and Lv 2010). Lasso could also run into inconsistency issues when the variables are highly correlated (Zou and Hastie 2005). We used 10-fold cross validation to select the smoothing parameter when we carried out Lasso regression (see Tibshirani (1996) and Friedman et al. (2010) for more details).

**Sparse Partial Least Squares (sPLS):** Partial least squares seek to reduce the high-dimensionality issues of the design matrix in linear regression models through a latent matrix whose columns maximize the product of the linear correlation between predictors and responses and the variance of responses. The sPLS method further introduces sparseness to the partial least squares estimators by means of a $L_1$-penalty with a thresholding parameter, in order to avoid inconsistency problems when there
are a substantial number of noisy covariates (Chun and Keleş, 2010; Chung et al., 2013). However, this method is inefficient in measuring the statistical significance of whether the parameters associated to certain variables are effectively zero (Olson Hunt et al., 2014). In our implementation, the thresholding parameter involved in sPLS is estimated using a 10-fold cross-validation criteria.

**Sliced Inverse Regression (SIR) with CSS selection method:** In general, the SIR methods (Li, 1991; Duan and Li, 1991; Zhong et al., 2005; Li and Yin, 2008; Coudret et al., 2014; Weisberg, 2002, among others) reduce the excess dimension in a non-parametric setting through the estimation of the linear space spanned by the coefficients of the covariables, also known as *effective dimension reduction* (EDR) subspace. This subspace is obtained by an approximate eigenvalue decomposition that involves an estimation of the covariance matrices of the design matrix and the conditional expectation of the explanatory variables given the response. The estimation of the covariance matrix requires to partition the dependent variable into subgroups, called *slices*. The SIR method can capture both linear or nonlinear associations between the response and covariates. However, the estimation of the dimension reduction space does not actually lead to a variable selection procedure and the covariance estimation relies heavily on the homogeneity of the response within each slice (Wu et al., 2010). Because of this, we opt to incorporate the CSS (*Closest submodel selection*) variable selection procedure into the SIR method. Furthermore, to better deal with the fact that there is a larger number of covariates than observations, we employed the SIR-QZ algorithm, an upgrade of the SIR method based on the generalized Shur decomposition for undermined cases (Coudret et al., 2014, 2017). Finally, we studied the association between proxies and temperatures through a linear regression between the observed anomalies and a number of EDR directions, i.e., orthogonal basis of the EDR subspace, determined by marginal dimension tests (Cook, 2004).

**Principal Component Regression (PCR):** PCR simply means that we replace the original covariates by their PCs. To select how many and which PCs to use, we
fitted a regression model between the temperature and PCs of eight different sets of covariates selected in each of the eight different time periods based on the training data in calibration period. We then selected the number of PCs in each of the eight regressions as the minimum number that attains, for the first time, an adjusted $R^2$ of at least 70% in each case. PCR is often used when covariates are highly-correlated or when the number of covariates is larger than the number of observations. A caveat of this method is that the principal components with smaller contribution to variance are not necessarily the ones that associate less with the dependent variable in a linear regression model (Jolliffe, 1982; Tibshirani, 1996).

**Supervised Principal Components (sPCR):** Because of the above-mentioned caveat of directly using PCR, Bair et al. (2006) developed a technique where PCR is applied only to a certain subset of covariates that exhibits a considerable amount of association with the dependent variable, and the threshold of “considerable” is chosen through cross-validation. Compared to PCR, the sPCR ensures the dimensionality reduction on the covariates space while taking the association between the covariates and the dependent variable into account. In general, its performance is quite similar to sPLS method (Chung et al., 2013).

The data reduction allows us to fit linear regression models between temperatures and proxies. After we fit a linear regression model under each of the five data reduction methods and for each of the eight proxy groups listed in Table 1, we compute a single reduced proxy series following Barboza et al. (2014) for each group. All reduced proxies are shown in Fig. 3. These series are highly correlated, with the reduced proxies obtained by PCR standing out as least similar to the others by this metric (Fig. 4).

3.2. **Model Specification.** As we emphasized in the introduction, we use BHM for our problem. The first level of a BHM always models the likelihood of the data (Tingley et al., 2012). The second level models the temperature process, where forcings may be included to improve the reconstruction (Barboza et al., 2014; Li et al., 2010), since they are known to drive the temperature process. An additional benefit is that this allows to attribute forcings
(i.e., determine causality, Hegerl and Zwiers, 2011) as part of the inference procedure. However, this raises the spectre of overfitting, whereby the model would discount the noisy proxy data and place undue influence on the forcings, and not enough on internal variability. To avoid this risk, it may be preferable to model temperature fluctuations as a smooth function of time (say, via splines) without including forcings, then perform forcing attribution on the inferred temperature posterior Schurer et al. (2013a,b), which guarantees independence: this way, if the reconstruction bears a strong resemblance to the forcings, it is only because the
latter are reflected in the values of the predictors, not because they were fed to the model. In this section we explore both end-members, as well as an intermediate case.

Below we first define notations for our models:

- \( RP_i^t \): \( i \)-th reduced proxy at time \( t \).
- \( T_t \): temperature anomaly at time \( t \).
- \( \tilde{C}_t = \log(C_t) \): Transformed greenhouse gases. The log transformation is chosen to approximate the radiative forcing due to changes in the equivalent CO\(_2\) concentration (Barboza et al., 2014).
- \( \tilde{V}_t = \log(-V_t + 1) \): Transformed volcanic forcing. See more details in Barboza et al. (2014) for the choice of the transformation.
- \( B_k^{k,\tau}_t \): \( k \)-th B-Spline basis function at time \( t \) with a uniform knot sequence \( \tau \) (de Boor 2001; Ramsay and Silverman 2005). Here we choose cubic B-spline bases and we denote \( K(\tau) \) as the total number of basis elements.

We then define the first level of BHM as

\[
RP_i^t = \alpha_0^i + \alpha_1^iT_t + \epsilon_i^t,
\]

where \( \{ \alpha_j^i \} \) are intercepts \((j = 0)\) and slopes \((j = 1)\) for \( i = 1, \ldots, N \), and \( \epsilon_i^t \) are normally-distributed random variables with finite variances \( \{ \sigma_i^2 \} \). Note that in our case \( N = 8 \); the time variable \( t \) is defined on each nest according to the intervals of Table 1.

The second level will be defined in three different forms:

**No forcing (model "NF")**: The main idea of this model is to evaluate the central hypothesis of this article, that is, the paleoclimate reconstruction can perform well without taking into account the external forcings, as long as a smoothing function has been included to approximate the dynamic behavior of the temperature series. We do so as:

\[
T_t = \beta_0 + \sum_{k=1}^{K(\tau)} \beta_k B_k^{k,\tau}_t + \eta_t,
\]
where $\beta_k$ are coefficients for B-spline bases, and $\eta_t$ are also normally-distributed random variables with finite variances $\sigma^2_{\eta_t}$. For simplicity, the error terms $\epsilon^i_t$ and $\eta_t$ are assumed to be independent.

**With forcing (model "WF"):** In order to have a baseline model to evaluate Model NF, we define

$$T_t = \beta_0 + \beta_1 S_t + \beta_2 \tilde{V}_t + \beta_3 \tilde{C}_t + \eta_t. \quad (2)$$

Both first level and second level models are defined for $t = 1, \cdots, 2000$ (Common Era). It is important to add that Models NF and WF simply assume an independent error structure. This is because Barboza et al. (2014) found that complex error structures make little difference when forcings are added to the reconstruction.

"Mixed" Model: Finally we consider the more realistic case where temperature reflects both external forcings and internal dynamics. This model is a combination of equations (1) and (2), as follows:

$$T_t = \beta_0 + \beta_1 S_t + \beta_2 \tilde{V}_t + \beta_3 \tilde{C}_t + \sum_{k=1}^{K(\tau)} \gamma_k B^{k,\tau}_t + \eta_t. \quad (3)$$

where $\gamma_k$ are the coefficients for the B-Spline basis. This last case is of most obvious relevance to climate dynamicists. Indeed, it is common knowledge that Earth's temperature varies both as a result of internal causes (NF) and forcings (WF). It is thus most natural to set up a mixed model that reflects both causes. The downside is that the model is more complex, thus making estimation more challenging.

3.3. **Sampling with INLA.** The computational challenge of MCMC inference has been a concern for Bayesian paleoclimate reconstructions. It is crucial to overcome this computational bottleneck before we can move forward to a more complex space-time reconstruction. Here we introduce the INLA sampling strategy to accelerate the MCMC procedure, and we hope this experiment can serve as a template for employing INLA in more comprehensive models.
The INLA approach is applicable to a general specification for which the mean \( \eta_i \) of the observations \( y_i \) follows a linear structure:

\[
\eta_i = \alpha + \sum_{m=1}^{M} \beta_m x_{mi} + \sum_{t=1}^{L} f_t(z_{li})
\]

(4)

where \( \alpha \) represents an intercept, the coefficients \( \beta = (\beta_1, \ldots, \beta_M) \) relate \( M \) covariates \((x_1, \ldots, x_M)\) to \( \eta_i \), and \( f = \{f_1(\cdot), \ldots, f_L(\cdot)\} \) is a collection of random effects defined on a set of \( L \) covariates \((z_1, \ldots, z_L)\) (see Rue et al. (2009) and Blangiardo et al. (2013)). Denote the set of random variables as \( \theta = (\alpha, \beta, f) \) with \( K \) hyperparameters \( \psi = \{\psi_1, \ldots, \psi_K\} \), and the vector of observations as \( y = (y_1, \ldots, y_n) \). Model (4) leads to conditional independence of \( y \) given \( \theta \) and \( \psi \):

\[
p(y|\theta, \psi) = \prod_{i=1}^{n} p(y_i|\theta_i, \psi).
\]

In our models, if we consider \( y_i \) as the reduced proxies, \( \eta_i \) the linear mean of the reduced proxies, \( x_m \) the external forcings and/or the set of spline basis, and \( f(z_i) \) the latent variables (temperature anomalies in our case), then our models fall into the general specification of INLA.

The main objectives of our Bayesian estimation are to compute the marginal posterior distribution of each parameter in \( \theta \):

\[
p(\theta_i|y) = \int p(\theta_i, \psi|y) d\psi = \int p(\theta_i|\psi, y)p(\psi|y) d\psi
\]

To attain computational advantages, INLA approach assumes that (i) the prior of vector \( \theta \) is a multivariate normal random vector with a precision matrix that depends on hyperparameters \( \psi \), and (ii) the vector \( \theta \) is conditionally independent given the hyperparameters. These two assumptions specify \( \theta \) as a Gaussian Markov random field. INLA further substitutes the two components \( p(\psi|y) \) and \( p(\theta_i|\psi, y) \) by their approximations. The first component can be
approximated using a Laplace Approximation (see Tierney and Kadane (1986)):

\[
p(\psi|y) = \frac{p(\theta, \psi|y)}{p(\theta|y)} \propto \frac{p(\psi)p(\theta|\psi)p(y|\theta)}{p(\theta|\psi, y)}
\]

\[
\approx \frac{p(\psi)p(\theta|\psi)p(y|\theta)}{\tilde{p}(\theta|\psi)} \Bigg|_{\theta = \theta^*(\psi)} := \tilde{p}(\psi|y),
\]

where \(\tilde{p}(\theta|\psi, y)\) is the Gaussian approximation of \(p(\theta|\psi, y)\) and \(\theta^*(\psi)\) is its mode (see Rue et al. (2009)). The second component can be approximated in a similar way:

\[
p(\theta|\psi, y) = \frac{p((\theta_i, \theta_{-i})|\psi, y)}{p(\theta_{-i}|\theta_i, \psi, y)}
\]

\[
\approx \frac{p((\theta_i, \theta_{-i})|\psi, y)}{\tilde{p}(\theta_{-i}|\theta_i, \psi)} \Bigg|_{\theta_{-i} = \theta^*_{-i}(\theta_i, \psi)} := \tilde{p}(\theta_i|\psi, y),
\]

where \(\theta = (\theta_i, \theta_{-i})\), \(\tilde{p}(\theta_{-i}|\theta_i, \psi, y)\) is the Gaussian approximation of \(p(\theta_{-i}|\theta_i, \psi, y)\) and \(\theta^*_{-i}(\theta_i, \psi)\) is its mode. The approximation in (5) possesses good precision, but it is very time demanding because it requires to recompute \(\tilde{p}(\theta_i|\psi, y)\) for each value of \(\theta\) and \(\psi\). A more efficient approach is to use the simplified Laplace Approximation that is based on a Taylor’s expansion of \(\tilde{p}(\theta_i|\psi, y)\) in (5). As mentioned in Rue et al. (2009) and Blangiardo et al. (2013), INLA first explores the marginal joint posterior of the hyperparameters \(\tilde{p}(\psi|y)\) in order to locate the mode and then performs a grid search to produce a set of “relevant” points \(\{\psi^*\}\) together with a set of weights \(w_{\psi^*}\) as an approximation of this marginal distribution. The marginals \(p(\psi^*|y)\) are then refined using interpolation methods. Finally, the marginals \(\tilde{p}(\theta_i|y)\) are obtained as follows:

\[
\tilde{p}(\theta_i|y) \approx \sum_{\psi^*} \tilde{p}(\theta_i|\psi^*, y)\tilde{p}(\psi^*|y)w_{\psi^*}.
\]

3.4. Priors. The models proposed in section 3.2 were implemented using the R package r-inla (www.r-inla.org). The implementation followed the methods provided in Ruiz-Cárdenas et al. (2012) and Muff et al. (2015) on the use of the INLA methodology in state-space models, dynamic linear models, and in general models whose mean can be written into equation (4).
These methods together with Martins et al. (2013) allow INLA to be applicable to a wide array of Bayesian models such as BHM that consists of several layers.

As Bayesian estimation, INLA requires priors for unknown parameters. Below is the list of priors we used in our models:

- $\alpha_i^j \sim N(0, 3), \beta_\ell \sim N(0, 3)$ for $i = 1, \ldots, N$, $j = 0, 1$, and $\ell = 0, \ldots, 3$ for Model WF and $\ell = 0, \ldots, K(\tau)$ for Model NF. The choice of the variance is completely arbitrary, but the main idea is to select a relatively large one.
- $\rho_i := -\log \sigma_{\epsilon_i}^2 \sim \text{log-gamma}(1, 10^{-20})$ (very small precision) for $i = 1, \ldots, N$.
- $\rho_0 := -\log \sigma_{\eta}^2 \sim \text{log-gamma}(1, 10^{-20})$ (very small precision).

4. Results.

In the following, the results presented use model WF for comparison with Barboza et al. (2014), unless otherwise specified.

4.1. Impact of data reduction choices. As a first exercise, we analyze the change in the predictive capacity of the reconstruction model when more equations involving proxies are included. We used two proper scoring rules Gneiting and Raftery (2007) as measures of predictive ability: the Interval Score at $\alpha$ level ($\text{IS}_\alpha$) and the Continuous Ranked Probability Score (CRPS). These scores have been previously employed in the verification of point forecasts in environmental sciences for example, as well as the area of paleoclimatic reconstructions (see Barboza et al. (2014) and Scheuerer (2014)). Table 2 contains the predictive measures using the INLA’s prediction intervals and the observed anomalies over 1850-1899 as an out-of-sample validation interval. The last column consists of the mean square error (MSE) between the smoothed reconstruction and the borehole-based reconstruction of Pollock and Smerdon (2004) over 1600-1899 as an out-of-sample validation interval. Smoothing was accomplished through a Butterworth low-pass filter with a 50-year cutoff and order equal to 4. We compared in this case Model WF with a single RP (the longest available) with respect to model WF using the 8 available reduced proxies, where the comparison was made under the five dimension reduction methods explained above.
It is evident that there is an improvement in all the measures when we use all the available reduced proxies over the case \( N = 1 \), under the methods SPLS, PCR and sPCR for the first validation period. For the PS04 dataset validation, all the methods except SIR shows an improvement in terms of MSE. (Table 2, last column). Also note that, among the models with external forcings, the techniques that best results from the viewpoint of these prediction measures are obtained with sPCR and PCR.

### Table 2. Comparison of predictive measures.

| Model | \( N \) | Method | \( IS_{80} \) | \( IS_{95} \) | CRPS | MSE  |
|-------|--------|--------|--------------|--------------|------|------|
| WF 1  | PCR    | 0.4678 | 0.1792 | 0.1641 | 0.1476 |
| WF 1  | sPCR   | 0.5821 | 0.2146 | 0.2593 | 0.2134 |
| WF 1  | LASSO  | 0.4658 | 0.1780 | 0.1655 | 0.1744 |
| WF 1  | sPLS   | 0.4749 | 0.1813 | 0.1810 | 0.1647 |
| WF 1  | SIR    | 0.4779 | 0.1819 | 0.1671 | 0.1692 |
| WF 8  | PCR    | 0.2493 | 0.0840 | 0.0986 | 0.0392 |
| WF 8  | sPCR   | 0.1969 | 0.0719 | 0.0745 | 0.0926 |
| WF 8  | LASSO  | 0.5044 | 0.3128 | 0.1559 | 0.1735 |
| WF 8  | sPLS   | 0.3436 | 0.1687 | 0.1177 | 0.1579 |
| WF 8  | SIR    | 0.6485 | 0.4797 | 0.1871 | 0.2124 |
| NF 8  | PCR    | 0.2966 | 0.0958 | 0.1249 | 0.0275 |
| NF 8  | sPCR   | 0.4275 | 0.1624 | 0.1600 | 0.0249 |
| NF 8  | LASSO  | 0.5434 | 0.3545 | 0.1644 | 0.1828 |
| NF 8  | sPLS   | 0.2617 | 0.0942 | 0.0967 | 0.1326 |
| NF 8  | SIR    | 0.5772 | 0.3955 | 0.1720 | 0.1964 |
| Mixed 8 | PCR | 0.3509 | 0.1101 | 0.1579 | 0.0240 |
| Mixed 8 | sPCR | 0.3660 | 0.1368 | 0.1357 | 0.0249 |
| Mixed 8 | LASSO | 0.5291 | 0.3385 | 0.1613 | 0.1791 |
| Mixed 8 | sPLS | 0.3131 | 0.1404 | 0.1101 | 0.1495 |
| Mixed 8 | SIR  | 0.5986 | 0.4209 | 0.1766 | 0.2019 |

4.2. **Impact of Model Choice.** We are also interested in assessing whether a linear combination of B-spline bases can model GMST without the inclusion of external forcings at all. It is clear from equations (1) and (3) that one of the drawbacks of Models NF and Mixed is the arbitrariness of \( K(\tau) \). We analyze the relationship between the temperature observed during the calibration period (1900-2000) and a linear combination of BSplines. The number of bases in Model NF is selected according to the adjusted \( R^2 \) of a linear regression model between observed anomalies and the corresponding basis functions. Based on the above,
Figure 5. Paleoclimate Reconstruction in the Common Era (CE) with 95% prediction bands. Best two choices per validation method.

we selected 6 BSpline functions for this period and we take \( K(\tau) = 120 \) based on the assumption that the number of BSpline bases is uniform throughout the entire reconstruction period. Note that the high prevalence of annually-resolved proxy data allows to assume that a constant number of BSpline bases might be adequate to describe the temperature mean.

The choice of \( K(\tau) = 100 \) for model Mixed is based on the same criteria as before. Finally, we fit the models NF and Mixed with the previous choices of \( K(\tau) \), using the five different data reduction techniques described in section 3.1. These results are also shown in Table 2. Note that the SPLS method achieves a better performance in terms of the predictive measures for the first validation period, and PCR gets the smallest MSE for the second period.

Four reconstructions of Common Era GMST are shown in Figure 5. In order to illustrate the reconstruction that we obtained for both models, we considered the best two choices in terms of the validation measures for the first out-of-sample period and the best two choices for the second testing period. sPCR and PCR methods for both WF and Mixed models are the best choices according to the two testing periods.
The best model for the first testing period (sPCR-WF) shows an interesting balance in terms of the variance of the reconstructed series and the width of the confidence region approximated by INLA. The remaining 3 reconstructions show similar small-scale tendencies with respect to the best choice, but the width of their confidence regions is greater. A closer look of the reconstructions is shown in Figure 6, where the first testing period appears between the red lines. Note that sPCR-WF closely predicts the anomalies observed in the first testing period and it does so with a higher level of accuracy than the remaining reconstructions. In addition, the other three reconstructions underestimate in an almost analogous way the anomalies observed during the same period. At least for this validation exercise there is not a clear advantage of using a B-Spline basis as an additional linear term in equation (3).

Figure 7 shows a comparison of the smoothed reconstructions using a low-pass filter and the borehole-based reconstruction of Pollack and Smerdon (2004) (PS04 dataset). In this case, the mixed versions of the sPCR and PCR models with external forcings provide the best adjustment in terms of the MSE measure, especially during the 1700-1850 period. We
4.3. **Impact of INLA sampling.** We now quantify the trade-offs of approximating the MCMC procedure using INLA. The WF model in its simplest case (1 nest) was fitted in Barboza et al. (2014) using an MCMC approach. We employed this approach in order to adjust the WF model with the first reduced proxy from the sPCR method (we chose this method just for comparison purposes). The MCMC was performed using the same priors as in Barboza et al. (2014), but with a larger calibration period (1900-2000). The results are shown in Figures 8 and 9. Note that the MCMC reconstruction reaches cooler temperatures than INLA’s and the MCMC confidence bands along the reconstruction period are narrower. This last fact coincides with a small difference in terms of the interval score measure. Despite these contrasts, the general trends of both reconstructions are quite similar.

Another point of comparison is the estimated coefficients of the external forcings in equation (2). The estimated density function for each coefficient is shown in Figure 9. The
behavior of the estimated parameters of the three external forcings is very similar between the two methods: by far the most influential external forcing in both reconstructions is the greenhouse gas component, followed by explosive volcanism. Consistent with Schurer et al. (2013b), solar irradiance comes last, and is indistinguishable from a zero effect.

For the same reason that we explained above, the estimated density function of the CO\(_2\) coefficients are more concentrated when we use an MCMC algorithm, to a lesser extent for the rest of the coefficients. This behavior confirms the observed details of Figure 8.

In terms of computational efficiency, the INLA procedure is quite remarkable, not only for our case but in most of the previous work on a similar topic as well (see Rue et al. (2009), Blangiardo et al. (2013), Ruiz-Cárdenas et al. (2012) for a few examples). The computational cost of MCMC sampling with 5000 samples was approximately 8 hours, whereas the computational time of INLA’s best model with a single reduced proxy was approximately 15 seconds. This comparison was performed on an Ubuntu 16.04 server with Intel Xeon E5-2630 (8-cores, 2.40GHz) and 64 GB of RAM. This large speedup allowed us to explore a far wider variety of modeling choices than MCMC alone.
Figure 9. Posterior densities of $\beta_1$, $\beta_2$ and $\beta_3$ for Model sPCR-SSwF and MCMC using PCR single reduced proxy.

4.4. Are we living in extraordinary times? Finally, we take advantage of our probabilistic output to ask whether the levels and rates of warming over the recent past are exceptional in a 2,000 year context. Fig. 10 compares the temporal means of the last 10, 25, 50 and 100 years of the record compared to all similar previous intervals. That is, for the 25y case, we compare the mean over 1976-2000 to the mean over 1951-1975, 1926-1950, and all other 25-year segments back to 1 CE. It is evident that in all four cases the most recent period appears detectably warmer than any other time in the past 2,000 years, which confirms and strengthens the original conclusions of Mann et al. (1999).

The situation is more nuanced for warming rates: there is no discernible difference on 10 or 20y intervals, but warming rates over 1951-2000 and 1901-2000 appear highly anomalous in a 2,000 year context. This is not surprising, as transient heat exchanges between the surface and deep ocean are known to occur on scales shorter than a few decades (Hansen et al., 2005). These transients average out over 50-100y scales, and reveal a highly anomalous warming rate, which can be unequivocally tied to the radiative forcing due to anthropogenic emissions of $CO_2$ (parameter $\beta_3$ in the WF and Mixed models).
5. Conclusions

We carried out a Bayesian inference of global mean surface temperature over the past 2,000 years. By leveraging INLA to lighten the computational burden, our framework allows us to investigate a wide range of model choices and data reduction strategies. We validated the result using instrumental data over the 1850-1899 period, and using independent borehole
temperature inversions over 1600-1899. The former validates the reconstruction precisely to an interannual scale, while the latter validates only the multi-decadal to centennial behavior.

Below are a few take-home messages:

- The data reduction techniques provide roughly equivalent results, with sPCR and PCR performing marginally better than other methods.
- The model choice is highly consequential. Model "Mixed" is the most physically justifiable, and it guarantees a balance between the validation measures on the first and second testing periods. This models also appears to perform at least as well as other choices. The additional nonparametric terms in the mean component of equation (3) allows us to capture long-memory behavior that is not included in the external forcings, which compensates for the independent structure of the errors.
- In cases where both INLA and MCMC are implemented, INLA allows to approximate the MCMC solution at a fraction of the computational cost, but with wider prediction intervals. This exercise was performed only for the simplest model available (1 reduced proxy), because of the prohibitive cost of the MCMC approach for more complex models like the ones presented in Figure 5.
- Adding to a wide body of literature, we find that current temperature levels are unprecedented in the past 2,000 years. The twentieth century also stands out as warming more rapidly than any other century in the past 2,000 years. All models that include forcings (WF, Mixed) show that the man-made increase in atmospheric carbon dioxide is the leading contributor to this warming effect.

One limitation of our analysis is the strong dependence of our results on the choice of the testing period. Ideally, a cross-validation exercise should be carried out to determine with greater certainty the expected prediction error of the models, but due to the restricted access to additional comparison information the cross-validation is very challenging for this problem. Another way to improve our current study is to consider the space-time variability of the reduced proxies and temperatures in the model. Since INLA has been proven
to be computationally efficient, it could be used to extend our studies to spatiotemporal reconstructions of surface temperature.

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