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# Pairwise Scale-Space Comparison of Time Series with Application to Climate Research

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Abstract. In this paper, we study how sea surface temperature varia-11 tions in the North Atlantic and the Norwegian Seas are correlated with the 12 climate in the Northern Hemisphere in late Holocene. The analysis is per-13 formed by testing statistical hypotheses through novel scale-space method-14 ologies. In late Holocene, the proposed techniques reveal that the climate de-15 velopment in the subpolar North Atlantic has been incoherent with the de-16 velopment in the Norwegian Sea and the Northern Hemisphere. A prominent 17 discrepancy between the three analyzed series is identified for the periods 18 associated with the Medieval Warm Period and the Little Ice Age. A diver-19 gence between the oceanic series and the global Northern Hemisphere tem-20 perature estimate detected in the  $20^{th}$  century is in line with the inferred im-21 print of recent climate change which suggests accentuated warming in par-22

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 $_{\rm 23}$   $\,$  ticular over continental regions. Overall, the results obtained by scale-space

<sup>24</sup> analysis underscores the significance of the northern North Atlantic in shap-

<sup>25</sup> ing the climate globally, mainly through changes in the strength and struc-

<sup>26</sup> ture of the Atlantic meridional overturning circulation.

# 1. Introduction

A best possible understanding of present and past climate is of utmost 27 importance for producing reliable predictions of future climate scenarios. 28 Today we face changes in the climate all over the world and the observed 20 changes at different locations can show large discrepancies. Here we focus 30 on a particular area of interest by investigating how the trends in sea 31 surface temperature (SST) in the North Atlantic and the Nordic Seas are 32 related with the climate development in the Northern Hemisphere during 33 late Holocene. 34

To gain insight into this question, we utilize the theory [e.g. *Bjerknes*, 35 1964] that variability of SST in the North Atlantic and the Nordic Seas 36 has a profound effect on climate in the Northern Hemisphere due to heat 37 release to the atmosphere from the North Atlantic Current (NAC). The 38 NAC plays an important role in the Atlantic Meridional Overturning Cir-39 culation (AMOC), which is an essential component of the global climate 40 system [Wellinga and Wood, 2002], transporting heat northward via the 41 NAC and ventilating the world ocean through the North Atlantic Deep 42 Water (NADW) formation. The AMOC and regional climate are closely 43 linked [e.g. Latif et al., 2004] and known to vary in a broad range of time-44 scales [e.g. *Thornalley et al.*, 2009]. The short-term variability is primarily 45 driven by the atmosphere [Marshall et al., 2001], whereas at longer time-46

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scales, the role of the ocean becomes more important [e.g. *Bjerknes*, 1964;

<sup>48</sup> Timmermann et al., 1998; Knight et al., 2005].

Historical records and proxy climate data from the Northern Hemisphere 49 have provided evidence for the most recent major climate anomalies, such 50 as the warm Medieval Warm Period (MWP) between 800 and 1400 AD 51 [e.g. Lamb, 1965; Bradley et al., 2003; Mann and Jones, 2003; Berner et 52 al., 2011], and the following colder era, the Little Ice Age (LIA) between 53 1400 and 1900 AD [Grove, 1988; Bradley and Jones, 1993; Moberg et al., 54 2005; Mann et al., 2008]. Several theories have been proposed to explain 55 the possible cause for these anomalies, such as long-term variability in 56 total solar irradiance [Shindell et al., 2001], sulfate aerosols ejected into 57 the atmosphere by volcanism [Crowley, 2000], and changes in large-scale 58 ocean circulation [Broecker, 2000; Crowley, 2000].

The aim of this paper is to analyze the SST variability in the subpo-60 lar North Atlantic and the Nordic Seas in late Holocene and to obtain a 61 better understanding of how the variability in these SSTs correlates with 62 the Northern Hemisphere temperatures. We start out by performing a 63 statistical comparison of two 1200-year-long SST proxy records from the 64 Reykjanes Ridge, in the subpolar North Atlantic, and the Vøring Plateau, 65 in the Norwegian Sea. Specifically, we want to test whether there have 66 been different climatological developments at the Reykjanes ridge and the 67 Vøring plateu for the last 1200 years of the Holocene. If such differences 68 are found we would like to give a characterization of when and at what 69

time scales they have occurred. In addition, we would like to test if there 70 are occasions where changes at both locations have been of the same type, 71 but one has changed more rapidly than the other. Moreover, we would like 72 to give a good characterization of how these two SST series relate to the 73 Northern Hemisphere temperature, presented by Mann et al. [2008], for 74 the same time period. Such exploratory data analyses can give new insight 75 into the interpretation of the climatological phenomena observed during 76 this period. 77

New insights into the phenomena underlying these data sets can be ob-78 tained using the methods of time series analysis [e.g. Box and Jenkins, 79 1970; Brockwell and Davis, 1991 and Shumway and Stoffer, 2000]. A de-80 tailed description of the data sets analyzed will be given in Section 4 but 81 an important difference between the three time series should be noted al-82 ready here, namely that the Northern Hemisphere data set is sampled on a 83 regular grid as five year means while the two SST series are unevenly sam-84 pled. We note that compared to the extensive literature on the analysis of 85 evenly sampled signals, fewer papers address unevenly sampled series, e.g. 86 Lomb [1976] and Scargle [1982]. Many of the methods for unevenly sampled 87 data are based on interpolation [e.g. Quahabi et al., 1998; Dowski, 1998]. 88 An alternative approach, frequently used for nonstationary signals, is to 80 explicitly or implicitly use sliding windows, such as short-time FFT and 90 time-varying multitaper methods, see e.g. Bayram and Baraniuk [2000] 91 and Thomson [2000]. 92

Recently, an important focus in time series analysis has been analysis on 93 several time horizons or scales. A pioneering scale-space analysis of den-94 sities and regression curves was given by *Chaudhuri and Marron* [1999]. 95 Their work has in recent years been extended to a large number of situa-96 tions, see e.g. Godtliebsen et al. [2002, 2003, 2004], Park et al. [2004, 2007], 97 Erästö and Holmström [2005, 2007], Hannig and Lee [2005], Hannig and 98 Marron [2006] and Olsen et al. [2008]. For more references on statistical QC scale-space methods, see *Holmström* [2010a] for a recent review. We view 100 scale-space methods as particularly useful in climatology since the salient 101 features in a time series may depend heavily on the time horizon it is ana-102 lyzed on. Scale-space methodologies have in recent years become a useful 103 tool also for geologists, glaciologists and oceanographers; see e.g. Berner 104 et al. [2008] and Miettinen et al. [2011]. 105

A pairwise scale-space comparison of time series was given by Park and 106 Kang [2008]. Here, we develop a technique which is similar to their ap-107 proach but there are two important differences. First, we compare slopes 108 instead of means since that is more natural in climatology where time-series 109 may exhibit non-stationary behavior with persistent changes in the mean 110 value. Second, we describe methods based both on classical statistical and 111 Bayesian ideas whereas *Park and Kang* [2008] give a procedure motivated 112 from a classical point of view only. The motivation for introducing the 113 Bayesian approach is to see whether two different statistical paradigms 114 give essentially the same results for the data sets analyzed. Such an agree-115

ment would be reassuring, bolstering the credibility of the results obtained.
Another reason for introducing the Bayesian approach is that, in a scale
space context, it can more easily handle complexities such as serial correlation in the time series. The classical scale space methodology used in the
comparison is still important, not least because of its much lower threshold
for new users.

The paper is organized as follows. In Section 2, we describe our 122 statistical model and give a short outline of the scale-space idea. In 123 Section 3, a description of the methodologies developed for pairwise 124 comparison of time series is given. A description of the climatologi-125 cal data and the results obtained are given in Section 4. A discussion 126 is provided in Section 5. An Appendix contains many of the details 127 of the Bayesian approach. Matlab functions used for our analyses can 128 be downloaded from http://www.unc.edu/~marron\_software.html 129 and http://mathstat.helsinki.fi/bsizer/. 130

## 2. Model, assumptions and scale-space background

Recall that our aim is a comparison of two time series. We assume that time series k, where k is 1 or 2, follows the simple model

$$y_{k,i} = m_k(x_{k,i}) + \sigma_k(x_{k,i})\varepsilon_{k,i}, \quad k = 1, 2; \quad i = 1, ..., n_k,$$
 (1)

where  $m_k$  and  $\sigma_k$  denote the unknown regression function and noise standard deviation function of time series k, respectively. The  $x_{k,i}$  denote the possibly unevenly sampled time points where observations  $y_{k,i}$  exist. Note

that the sampling in the two time series typically is not the same. The  $\varepsilon_{k,i}$  denote independently distributed random errors with mean 0 and variance 1. In the Bayesian model the errors are assumed to be Gaussian with possible correlations within each time series. There are  $n_k$  observations in time series k. In the data analyses considered in this paper,  $m_k(x_{k,i})$  is the true past temperature at time  $x_{k,i}$ ,  $y_{k,i}$  is its proxy-based reconstruction, and  $\sigma_k(x_{k,i})\varepsilon_{k,i}$  represents the error in the reconstruction.

For convenience of the reader, we next describe briefly the idea in scalespace methodologies. The notion of "scale" in our scale-space analyses always refers "time-scale". However, the methods developed could conceivably be applied also in other situations, such as in analysis of spatial data where features in different spatial scales would be of interest.

To keep things simple, we assume that we have observed just one time 146 series following the model in equation (1). A traditional analysis will search 147 for the underlying true m through a "smooth" estimate  $\hat{m}_h$  where the pa-148 rameter h controls the degree of smoothness. See e.g. Fan and Gijbels 149 [1996] for more details. Then, inference about m is based on  $\hat{m}_h$ . A major 150 disadvantage with this approach is that  $\hat{m}_h$  is a biased estimator of m. 151 The novel idea in a scale-space analysis is that we do not focus on the 152 search for the underlying true m. Instead, we study scale-space versions or 153 smooths of m, denoted by  $m_h$ . By this procedure, the estimators  $\hat{m}_h$  are 154 unbiased estimators of  $m_h$ . Hence, we avoid the bias problems that tradi-155 tional smoothing methods suffer from. Moreover, we avoid the search for 156

X - 10 GODTLIEBSEN ET AL.: SCALE-SPACE COMPARISON OF TIME SERIES an optimal smoothing level since in a scale-space analysis "all" scales are considered important. Similarly, in a Bayesian scale-space approach, inference is based on the distribution of the smooth  $m_h$ , given the observations  $y_i$ .

# 3. Pairwise Scale-Space Comparison

<sup>161</sup> In this section we describe two differently motivated scale-space method-<sup>162</sup> ologies for comparing two time series following the model given in Section 2.

## 3.1. A Classical Approach

Our approach here is a direct application of the original SiZer methodology developed by *Chaudhuri and Marron* [1999]. For time series k, at a particular point  $x_0$  and a given scale h,  $\hat{m}_{k,h}(x_0)$  is obtained by fitting the line

$$l(x) = \beta_{k,0} + \beta_{k,1}(x_0 - x)$$

locally to the data  $(x_{k,i}, y_{k,i})$ . In fact,  $\hat{m}_{k,h}(x_0) = \hat{\beta}_{k,0}$ , where  $(\hat{\beta}_{k,0}, \hat{\beta}_{k,1})$ minimizes

$$\sum_{i=1}^{n_k} [y_{k,i} - (\beta_{k,0} + \beta_{k,1}(x_0 - x_{k,i}))]^2 K_h(x_0 - x_{k,i}),$$
$$K_h(\cdot) = \frac{1}{h} K(\frac{\cdot}{h}),$$

and K is a kernel function, typically a symmetric probability density function. Here, we use a Gaussian kernel. The hypothesis we would like to test, for a given scale h, at the point  $x_0$ , is

$$H_0: \beta_{1,1}(x_0) = \beta_{2,1}(x_0)$$
 against  $H_1: \beta_{1,1}(x_0) \neq \beta_{2,1}(x_0).$ 

We do this by rejecting  $H_0$  if

$$\frac{|\hat{\beta}_{1,1}(x_0) - \hat{\beta}_{2,1}(x_0)|}{\widehat{\mathrm{SD}}(\hat{\beta}_{1,1}(x_0) - \hat{\beta}_{2,1}(x_0))} > q \tag{2}$$

where we use the plausible assumption

$$\operatorname{Var}(\hat{\beta}_{1,1}(x_0) - \hat{\beta}_{2,1}(x_0)) = \operatorname{Var}(\hat{\beta}_{1,1}(x_0)) + \operatorname{Var}(\hat{\beta}_{2,1}(x_0))$$

to estimate the denominator in equation (2), and q is a suitable quantile. The value of q is decided in the same way as in *Chaudhuri and Marron* [1999] with

$$\operatorname{ESS}_{h}(x_{0}) = \min\{\operatorname{ESS}_{1,h}(x_{0}), \operatorname{ESS}_{2,h}(x_{0})\}$$

where  $\text{ESS}_{k,h}(x_0)$  denotes the effective sample size of time series k for scale h and location  $x_0$ . The motivation for this approach is that it will be a conservative choice in the sense that we will have more confidence in the features found by our methodology.

In SiZer analyses the results of inferences are visualized with so-called 167 family plots and significance or feature maps, examples of which are shown 168 in Figure 1. In a significance map, a pixel (x, s) corresponding to time x and 169 scale  $s = \log_{10}(h)$  is colored blue or red depending on whether the slope 170 of the smooth of the true underlying temperature curve is significantly 171 positive or negative, respectively. Purple indicates non-significance and 172 pixels are colored gray if the data are too sparse to make any conclusions. 173 The SiZer maps for pairwise comparisons (middle panels of Figs. 2 - 4) are 174 interpreted analogously except now inferences are made on the slope of a 175

difference between two time series. The level of significance in all SiZeranalyses is 0.05.

## 3.2. A Bayesian Approach

The Bayesian approach is based on the BSiZer methodology described 178 in Erästö and Holmström [2005, 2007] and Holmström [2010b]. Denote 179 by  $\boldsymbol{y}_k = [y_{k,1}, \dots, y_{k,n_k}]^T$  the observed time series k, k = 1, 2. Let 180  $x_1 < x_2 < \cdots < x_n$  be a grid of time points where one wants to an-181 alyze the difference between the slopes of the smooths  $m_{1,h}$  and  $m_{2,h}$  of 182 the underlying unobserved curves. Let  $\boldsymbol{m}'_{k,h} = [m'_{k,h}(x_1), \dots, m'_{k,h}(x_n)]^T$ 183 be the vector of slopes of  $m_{k,h}$  computed on this grid. Our Bayesian scale 184 space analysis uses the posterior distribution of  $m{m}'_{1,h} - m{m}'_{2,h}$  given the data 185  $\boldsymbol{y}_1,\,\boldsymbol{y}_2$  to make inferences about the credible features in the difference be-186 tween the slopes of  $m_{1,h}$  and  $m_{2,h}$ , for a range of time scales h. As in the 187 classical SiZer approach, we also make an independence assumption about 188 the two time series which allows us to obtain a sample from this posterior 189 by sampling separately from the posterior distributions of  $m_{1,h}'$  and  $m_{2,h}'$ 190 and then simply subtracting the samples. The full details of the Bayesian 191 method are given in the Appendix. 192

An analog of a SiZer significance map can be obtained by choosing a credibility level  $0 < \alpha < 0.5$  and coloring a map pixel  $(x_j, s)$  corresponding to time  $x_j$  and scale  $s = \log_{10}(h)$  blue or red according to whether

$$P\left\{\boldsymbol{m}_{1,h}'(x_j) - \boldsymbol{m}_{2,h}'(x_j) > 0 \mid \boldsymbol{y}_1, \boldsymbol{y}_2\right\} \ge 1 - \alpha$$

or

$$P\{\boldsymbol{m}_{1,h}'(x_j) - \boldsymbol{m}_{2,h}'(x_j) < 0 \mid \boldsymbol{y}_1, \boldsymbol{y}_2\} \ge 1 - \alpha_1$$

and purple otherwise, where the probabilities are computed from the generated sample of slope differences. However, instead of using such pointwise inference, the maps are in fact drawn based on the joint posterior probabilities over the grid points  $x_j$ 's, where a method based on highest pointwise probabilities was used (cf. *Erästö and Holmström* [2005]). We have chosen  $\alpha = 0.05$  in all analyses.

<sup>199</sup> Note that we use the same symbol h for the scale space smoothing param-<sup>200</sup> eter both in the classical and the Bayesian methods although its technical <sup>201</sup> role in the two approaches is quite different. In the classical SiZer h is <sup>202</sup> the standard deviation (or width in the time domain) of the Gaussian ker-<sup>203</sup> nel used whereas in the Bayesian BSiZer it controls the roughness penalty <sup>204</sup> in spline smoothing (see the Appendix). Although a spline smoother can <sup>205</sup> be interpreted as an approximate kernel smoother, the relevant smoothing <sup>206</sup> scale ranges of the two methods have very different magnitudes.

## 4. Results

## 4.1. Data sets

The two SST series used in this study are diatom based August SST reconstructions with an uneven sampling resolution of 2 - 10 years from marine sediment cores Rapid 21-COM (hereafter Rapid) from the eastern flank of the Reykjanes Ridge, subpolar North Atlantic [*Miettinen et al.*, 2011; *Miettinen et al.*, 2012], and CR 948/2011 (hereafter CR) from the

Vøring Plateau, the Norwegian Sea [Andersen et al., 2004; Berner et al., 212 2011]. These two SST series were selected, because a) they represent the 213 highest-resolution SST reconstructions from the northern North Atlantic 214 for the last 1200 years, and b) they are located in critical areas in relation 215 to the NAC, which has an essential role on the North Atlantic climate, 216 i.e., core Rapid 21-COM is influenced by the western branch of the NAC 217 in the south of Iceland, and core CR948/2011 by the eastern branch of 218 the NAC in the Norwegian Sea. The SST reconstructions are based on 219 marine planktonic diatoms and transfer functions. Marine diatoms have 220 proven to be good indicators of surface water conditions in the region 221 [e.g. Koc-Karpuz and Schrader, 1990; Andersen et al., 2004; Berner et 222 al., 2008]. A training data set consisting of 139 surface samples with 52 223 diatom species and modern August SSTs from the Nordic Seas and the 224 North Atlantic [Andersen et al., 2004] was utilized to convert downcore 225 diatom counts to quantitative SST using the weighted averaging partial 226 least squares (WA-PLS) transfer function method [ter-Braak and Juggins, 227 1993]. The WA-PLS diatom transfer function has a RMSE of 0.75 °C, a 228 maximum bias of 0.44 °C and  $R^2$  of 0.96. More details can be found in 220 [Miettinen et al., 2011; Miettinen et al., 2012; Berner et al., 2011]. 230

The Northern Hemisphere surface temperature (hereafter NHem) reconstruction originally named as NH EIV Land+Ocean [*Mann et al.*, 2008]. It is based on a multiple proxy database consisting of tree-rings, marine sediments, speleothems, lacustrine sediments, ice cores, corals, and historical

GODTLIEBSEN ET AL.: SCALE-SPACE COMPARISON OF TIME SERIES X - 15 documentary series [*Mann et al.*, 2008]. This proxy database represents a significant extension of the database used in related earlier studies [*Mann et al.*, 1998, 1999; *Juckes et al.*, 2007]. See *Mann et al.* [2008] for further details about this data set.

# 4.2. Rapid

To get an idea about what significant features can be found in the Rapid 239 time series on different time scales, a SiZer analysis was performed and 240 the result is shown on the first row of Fig. 1. The immediate and overall 241 feature found is an increase in summer SST over the data set, manifested 242 by the color blue for all locations on scales covering the whole period. 243 A closer look at the feature map reveals some features at a centennial 244 time scale. At year 1000 AD, there is a significant increase in the SST 245 reconstruction while there is an abrupt decrease in the SST just after year 246 1700 AD. Furthermore, there is evidence in the data of a peak in the SST 247 around 1870 AD. This feature seems to be very clear and manifested on 248 scales ranging from 10 to 100 years. 249

#### 4.3. CR

From the SiZer analysis of the CR time series from the Vøring Plateau displayed in the middle row of Fig. 1, it is clear that, in contrast to the findings for the Reykjanes Ridge, there has been a decrease in temperature on time scales covering the whole period. On scales of length around 100 years, the temperature has decreased more abruptly around years 900,

<sup>255</sup> 1100, and 1400 AD. At scales of length 500 years, there is an increasing
<sup>256</sup> trend from around year 1500 AD to the present.

## 4.4. Nhem

In the last row of Fig. 1, the SiZer analysis reveals a millennial-scale 257 decrease in the surface temperature of the Northern Hemisphere. At scales 258 of 10 to 100 years, several features typically associated with major climate 259 transitions of the last Millennium are flagged as significant. In particular, 260 these are the peaks around years 850, 1050, and 1400 AD. A pronounced 261 temperature maximum centered at approximately 1050 AD corresponding 262 to the Medieval Warm Period (MWP, Lamb [1965]; Bradley et al. [2003]) 263 is detected as significant on scales up to 500 years which is a reflection of 264 a lasting positive surface temperature anomaly from around year 950 to 265 year 1100 AD. Finally, the SiZer map indicates that there is an abrupt 266 decrease in the temperature around year 1420 signifying the onset of the 267 Little Ice Age (LIA, Moberg et al. [2005]; Mann et al. [2008]). This is a 268 strong feature, visible at scales ranging from 10 to 200 years. 269

#### 4.5. Rapid vs. CR

By comparing the regional Rapid and CR summer SST reconstructions, we see that the two different methodologies yield very similar results (Fig. 272 2). Both approaches reveal that the record for Rapid has a significantly larger slope (blue color in Fig. 2) than the record for CR, i.e., in a long term perspective for the last 1200 years, the SST record for Rapid shows a clear

GODTLIEBSEN ET AL.: SCALE-SPACE COMPARISON OF TIME SERIES X - 17 warming trend compared with CR, which demonstrates a less pronounced 275 cooling tendency. On a shorter time scale, a blue area over a broad range 276 of scales can be seen around 1400 and 1800 AD showing the most distinct 277 periods when Rapid is increasing (warming) and CR decreasing (cooling). 278 Analysis of the maps displayed in Figs. 1 and 2 proves that the pairwise 279 scale-space comparison adds important knowledge about the characteristics 280 of the two time series. Note that around year 1800 AD the maps obtained 281 by separate analyses of Rapid and CR (Fig.1) are highlighted blue at a 282 broad range of time scales signifying the period of statistically significant 283 SST increase detected in both series. The pairwise comparison displayed 284 in Fig. 2 also show blue for some scales at this location. The implication 285 of this is that the temperature in Rapid is increasing significantly faster 286 than in CR, a fact that is not clear from the maps of the SiZer analyses of 287 Fig. 1 alone. 288

Finally, we note that the Bayesian approach reveals some features that 289 are not captured by the classical SiZer approach. The feature flagged 290 around 1200 AD is present only on very small scales. This potential event 291 occurs in the gray area of the classical approach, indicating that inference 292 cannot be performed with this methodology. The same can be stated 293 about the feature around 850 AD. For scales of length around 300 years, 294 the Bayesian approach flags a red area just before 1700 AD. By looking at 295 the observed data in the top panel of Figure 2, there is a vague indication 296 of increase in CR while Rapid is neither increasing nor decreasing. The 297

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## 4.6. Rapid vs. NHem

The comparison of a regional-scale Rapid and global NHem (Fig. 3) 301 series yields results qualitatively similar to the previous analysis between 302 Rapid and CR, indicating an increasing trend for Rapid and a decreasing 303 trend for NHem. Also, the most distinct periods of significantly different 304 temporal evolution of surface temperatures are evident at around 1400 and 305 1800 AD. However, the trends are reversed for the last century. Whereas 306 Rapid series shows slow cooling, NHem demonstrates a rapid warming 307 trend associated with anthropogenic forcing as indicated by a red area 308 over a broad range of scales. Moreover, a short period of cooling Rapid but 309 warming NHem can be seen around 1750 AD, which is not clear enough to 310 be flagged as significant by classical SiZer. It, however, appears as credible 311 in the Bayesian analysis, as indicated by the red area in the credibility 312 map. 313

From Figs. 1 and 3 it can be seen that around 1800 AD a similar phenomenon, as described for the comparison of Rapid and CR, is present. This means that also in the comparison of Rapid and NHem, it is clear that the pairwise scale-space comparison complements the information obtained by the two single time series scale-space analyses.

GODTLIEBSEN ET AL.: SCALE-SPACE COMPARISON OF TIME SERIES X - 19 In addition to the discrepancy observed around 1750, there are some other small differences between the classical and the Bayesian analyses but again, many of them occur at scales that are gray regions in the classical approach. Thus, overall, the agreement between the two approaches is remarkably good also in this case.

# 4.7. CR vs. NHem

The results obtained by comparing CR and NHem (Fig. 4) show dis-324 tinct differences compared with earlier combinations. First, the regional 325 temperature anomalies are more or less congruent with the global climate 326 development, e.g. the first part of the record until ca. 1400 AD is charac-327 terized by the highest SSTs in CR, as well as higher than average surface 328 temperatures in NHem. Secondly, in both reconstructions, the color purple 329 over a broad range of time scales indicates that the derivative is not found 330 to be significantly different from zero. This indicates that the slopes of CR 331 and NHem series in the considered temporal resolution are in phase for 332 most of the investigated period, i.e., they are characterized by a decreas-333 ing (cooling) long term trend for the last 1200 years. However, significant 334 differences can be seen in shorter time scales. Red color in a broad range 335 of scales from 800 to 1100 AD indicates a clear cooling trend for CR but 336 a lagged warming trend for NHem suggesting the northern North Atlantic 337 origin of the MWP. Similar periods of the regional surface temperature 338 evolution significantly different from the global climate development can 339 be seen around 1400 AD and in the last century. The opposite situation, 340

X - 20 GODTLIEBSEN ET AL.: SCALE-SPACE COMPARISON OF TIME SERIES <sup>341</sup> namely a stronger warming trend for CR can be seen from around 1500 to <sup>342</sup> 1750 AD.

By comparing Figs. 1 and 4, we infer again that the pairwise comparison 343 contributes additional information around years 900, 1400, and 1900 AD. 344 At approximately 900 and 1400 AD the single time series analyses show 345 a significant decrease of the surface temperature. Note, however, that the 346 pairwise comparison also flags red at this (these) position(s) suggesting that 347 the decrease in the regional CR surface temperature series is significantly 348 steeper than in NHem. After 1900, the separate analyses of CR and NHem 349 flag blue indicating significantly increasing temperatures. But, the increase 350 in CR series appears to be significantly slower than in NHem and the result 351 in the pairwise comparison map is therefore an area flagged as red. From 352 Figure 4 we can see again that for the comparison of these two data sets, 353 the two different statistical approaches show essentially the same feature 354 maps. 355

## 5. Discussion and conclusions

We have analyzed the pairwise differences in climate proxy time series using two statistical scale-space paradigms. The original SiZer technique uses classical, "frequentist" statistical reasoning based hypothesis testing while the BSiZer method is based on Bayesian inference that uses posterior probabilities. The regression models employed by the two approaches were also slightly different with SiZer assuming independent errors while BSiZer assumes Gaussian errors with possible temporal correlations. Further, SiZer

estimates errors from smoothing residuals while in the Bayesian setting one 363 is able to use prior knowledge e.g. in the form of estimated errors for the 364 reconstructions (cf. the Appendix). The strategies for simultaneous infer-365 ence or multiple hypothesis testing of features for sets of time points are 366 also different. Despite these contrasts, the two methods produce remark-367 ably similar feature analyses of pairwise differences in the reconstructed 368 temperature time series considered, a reassuring fact that increases our 360 confidence in the robustness of the results. We noted that many of the 370 differences in the feature maps actually occur at least partly in the gray 371 areas of the SiZer maps where this method is unable to produce results due 372 to lack of sufficient data. Here the combination of data and prior informa-373 tion helps the Bayesian method and explains the difference in the results. 374 Posterior analysis of the error covariance structure also suggests that the 375 simpler independent error model of SiZer is probably sufficient here, as the 376 posterior distributions of the off-diagonal elements of the error covariance 37 matrices were highly concentrated near zero. 378

The results from both statistical methods show statistically significant features from millennial to centennial time scales. The three analyzed series display regional-scale contrasts in climate development in the northern North Atlantic (CR SST vs. Rapid SST) as well as pronounced discrepancies between the regional and global-scale climate variations (North Atlantic records vs. NHem). We note that the difference in seasonal representation between the reconstructions can to some extent bias the inference

that follows from our analysis. One can expect, however, that due to the 386 longer time-scales mainly considered here, and because of the negligible 387 relative changes in seasonal orbital forcing over the analyzed 1200-year 388 long period when compared with the entire Holocene [e.g. Wanner et al., 389 2008, summer and annual mean temperature anomalies are in fact coher-390 ent. Besides, the estimate of the Northern Hemisphere surface temperature 391 is largely based on tree ring and latewood density data [e.g. Mann et al., 392 2008] which are reflective of summer conditions. This suggests that, just 393 like the SST reconstructions from the northern North Atlantic, the NHem 394 series may itself be biased towards the summer season. 395

A preliminary analysis of the results obtained underscores the signifi-396 cance of the northern North Atlantic in shaping the climate globally, mainly 397 through the changes in the strength and structure of the Atlantic merid-398 ional overturning circulation (MOC) [e.g. Latif et al., 2004; Manabe and 399 Stouffer, 1998]. A millennial scale progressive synchronous cooling demon-400 strated by the CR and NHem series until the end of the 1800s signifies 401 a lasting weakening of the eastern branch of the MOC associated with a 402 decreased influx of warm Atlantic waters northward to the Arctic via the 403 North Atlantic Current [Thornalley et al., 2009]. Although the relative 404 roles of various causal factors, both external and internal, behind these 405 changes are still controversial, it had to involve major reorganization in 406 oceanic and atmospheric circulation [e.g. Trouet et al., 2009; Mann et al., 407 2009]. 408

In shorter, centennial to multicentennial time scales, CR SST series from 409 the Norwegian Sea tends to lead NHem temperatures as can be inferred 410 from the earlier termination of the MWP (flagged red between ca 900-411 1100 AD in Fig. 4). A delayed response of ca. 50 years to decreasing 412 SST registered in CR in the Norwegian Sea also characterizes the onset 413 of the LIA in the NHem series (Fig. 4) at around 1450 AD. We note 414 that the origin of this lag could be related to a delayed shift in the North 415 Atlantic Oscillation (NAO) phase in response to persistent anomalies in 416 regional sea surface temperatures [e.g. Trouet et al., 2009; Swingedouw et 417 al., 2010; Miettinen et al., 2012]. It is notable that during the LIA, CR 418 series shows generally negative SST anomalies superimposed on a positive 419 trend which is steeper than the one observed in the NHem series (flagged 420 blue during 1500-1800 AD in Fig. 4). This (colder, but warming SST) 421 could suggest that NHem temperatures respond to rising SST only after 422 passing a threshold in the ocean-atmosphere system. 423

Rapid summer SST series displaying a persistent positive trend through-424 out the considered time interval seems to stand apart from the variability 425 recorded in CR and NHem records. *Miettinen et al.* [2012] however sug-426 gested that the observed statistically significant opposite climate tenden-427 cies between the sites in the subpolar North Atlantic and the Norwegian 428 Sea is a surface expression of the lasting changes in the relative strength 429 of the eastern and western branches of the MOC, with a possible ampli-430 fication through an atmospheric feedback. This apparent SST seesaw in 431

the northern North Atlantic might have an effect on two major anomalies of the European climate of the past Millennium: MWP and LIA. During the MWP, warming of the sea surface in the Norwegian Sea occurred in parallel with cooling in the northern subpolar North Atlantic, whereas the opposite pattern emerged during the LIA.

A divergence between the series detected in the  $20^{th}$  century is in line 437 with the inferred imprint of the recent warming which is generally associ-438 ated with anthropogenic forcing. Both instrumental data and model based 439 studies agree on accentuated warming in particular over continental re-440 gions [e.g. Karoly and Wu, 2005; Knutson et al., 2006; Trenberth et al., 441 2007]. A less pronounced oceanic SST increase is likely to be related to 442 greater evaporation and its heat storage. The recent atmospheric circula-443 tion changes, in particular a more positive NAO phase, may also contribute 444 to a moderation of warming trends in subpolar North Atlantic, specifically 445 in the Rapid core region, in the winter half-year. One should also note 446 a distinctive seasonality of the warming pattern with maximum warming 447 in winter and spring [Knutson et al., 2006] which is most likely another 448 forcing factor for a much steeper slope revealed in the NHem record in the 440 twentieth century. 450

## Appendix A: Details of the Bayesian Approach

## A1. The model

Write (1) in the form  $y_{k,i} = m_k(x_{k,i}) + \varepsilon_{k,i}$ , hence absorbing the variances in the variables  $\varepsilon_{k,i}$ . Denote  $\boldsymbol{\varepsilon}_k = [\varepsilon_{k,1}, \dots, \varepsilon_{k,n_k}]^T$  and, as a slight exten-

GODTLIEBSEN ET AL.: SCALE-SPACE COMPARISON OF TIME SERIES X - 25 sion of the model (1), assume that  $\boldsymbol{\varepsilon}_k \sim \mathrm{N}(\mathbf{0}, \boldsymbol{\Sigma}_k)$ , where  $\boldsymbol{\Sigma}_k$  is a general covariance matrix that allows the errors to be correlated. The likelihood of  $\boldsymbol{y}_k$  is then the Gaussian

$$p(\boldsymbol{y}_k|\boldsymbol{m}_k,\boldsymbol{\Sigma}_k) \propto |\boldsymbol{\Sigma}_k|^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\boldsymbol{y}_k-\boldsymbol{m}_k)^T \boldsymbol{\Sigma}_k^{-1}(\boldsymbol{y}_k-\boldsymbol{m}_k)\right),$$

where  $\boldsymbol{m}_k = [m_k(x_{k,1}), \dots, m_k(x_{k,n_k})]^T$ . We assume an inverse Wishart prior for  $\boldsymbol{\Sigma}_k$ ,

$$p(\boldsymbol{\Sigma}_k) \propto |\boldsymbol{\Sigma}_k|^{-(\frac{\nu_k+n+1}{2})} \exp\left(-\operatorname{tr}(\boldsymbol{W}_k \boldsymbol{\Sigma}_k^{-1})\right),$$
 (A1)

where the scale matrix  $\boldsymbol{W}_k$  is of the homoscedastic form  $\sigma_k^2 \boldsymbol{I}$  and the degrees of freedom  $\nu_k$  is selected so that the prior is rather uninformative.

For  $\mathbf{m}_k$  we use a prior that penalizes for roughness in the second derivative of the smooth underlying curve  $m_k$ . This idea can be conveniently implemented by assuming that  $m_k$  is a natural cubic spline, i.e., a twice continuously differentiable curve that consists of cubic polynomial pieces [e.g. *Green and Silverman*, 1994]. Thus, let the interval [a, b] contain the points  $x_{k,i}$ ,  $i = 1, \ldots, n_k$ . The spline  $m_k$  is then uniquely determined by its values  $\mathbf{m}_k$  at the knot sequence  $x_{k,1}, \ldots, x_{k,n_k}$  because these values determine the interpolating spline uniquely. The prior we use for  $\mathbf{m}_k$  is the improper Gaussian density

$$p(\boldsymbol{m}_k|\kappa_k) \propto \kappa_k^{\frac{\boldsymbol{n}_k-2}{2}} \exp\left(-\frac{\kappa_k}{2}\boldsymbol{m}_k^T \boldsymbol{L}_k \boldsymbol{m}_k\right),$$
 (A2)

where  $\boldsymbol{L}_k$  is a matrix such that

$$\boldsymbol{m}_k^T \boldsymbol{L}_k \boldsymbol{m}_k = \int_a^b [m_k''(x)]^2 \mathrm{d}x$$

and  $\kappa_k > 0$  controls the level of roughness penalty. The parameter  $\kappa_k > 0$ can be fixed or one can consider it unknown and in that case we specify a Gamma prior for it.

The joint posterior  $p(\boldsymbol{m}_k, \boldsymbol{\Sigma}_k, \kappa_k | \boldsymbol{y}_k)$  given the data  $\boldsymbol{y}_k$  is now obtained from Bayes' theorem,

$$p(\boldsymbol{m}_k, \boldsymbol{\Sigma}_k, \kappa_k | \boldsymbol{y}_k) \propto p(\boldsymbol{\Sigma}_k) p(\boldsymbol{m}_k | \kappa_k) p(\kappa_k) p(\boldsymbol{y}_k | \boldsymbol{m}_k, \boldsymbol{\Sigma}_k).$$
(A3)

We assume that the observations  $\boldsymbol{y}_1$  and  $\boldsymbol{y}_2$  are conditionally independent given the underlying curves  $\boldsymbol{m}_1, \boldsymbol{m}_2$ , and other model parameters and that, for the two time series, these parameters also are independent *a priori*. Then the triples  $(\boldsymbol{m}_1, \boldsymbol{\Sigma}_1, \kappa_1)$  and  $(\boldsymbol{m}_2, \boldsymbol{\Sigma}_2, \kappa_2)$  are independent given the data  $\boldsymbol{y}_1, \boldsymbol{y}_2$ ,

$$p(\boldsymbol{m}_1, \boldsymbol{\Sigma}_1, \kappa_1, \boldsymbol{m}_2, \boldsymbol{\Sigma}_2, \kappa_2 | \boldsymbol{y}_1, \boldsymbol{y}_2) = p(\boldsymbol{m}_1, \boldsymbol{\Sigma}_1, \kappa_1 | \boldsymbol{y}_1) p(\boldsymbol{m}_2, \boldsymbol{\Sigma}_2, \kappa_2 | \boldsymbol{y}_2).$$

We can therefore obtain a sample from the posterior  $p(\boldsymbol{m}_1, \boldsymbol{m}_2 | \boldsymbol{y}_1, \boldsymbol{y}_2)$  by 456 using Gibbs samplers to generate samples separately from  $p(\boldsymbol{m}_1, \boldsymbol{\Sigma}_1, \kappa_1 | \boldsymbol{y}_1)$ 457 and  $p(\boldsymbol{m}_2, \boldsymbol{\Sigma}_2, \kappa_2 | \boldsymbol{y}_2)$  and keeping only the parts that correspond to  $\boldsymbol{m}_1$  and 458  $\boldsymbol{m}_2$ . To get a sample of the slope vectors  $\boldsymbol{m}'_{k,h} = [m'_{k,h}(x_1), \ldots, m'_{k,h}(x_n)]^T$ 459 of the smooth  $m_{k,h}$  of the curve  $m_k$  one first smooths the sample of the  $\boldsymbol{m}_k$ 's 460 by multiplying the sample vectors by the matrix  $(I + hL_k)^{-1}$ , effectively 461 a discrete spline smoother. This produces a sample of smooths  $\boldsymbol{m}_{k,h}$  = 462  $[m_{k,h}(x_{k,1}),\ldots,m_{k,h}(x_{k,n_k})]^T$  and a second multiplication by an appropriate 463 matrix then produces a sample of the slope vectors  $\boldsymbol{m}_{k,h}'$  (cf. Green and 464 Silverman [1994]). Finally, a sample from the posterior distribution of the 465

slope difference  $m'_{1,h} - m'_{2,h}$  is obtained by forming pairwise differences between samples of  $m'_{1,h}$  and  $m'_{2,h}$ .

## A2. Selection of priors

The classical SiZer estimates the errors in (1) from residuals of the smoothed time series. In the Bayesian setting one tries to utilize any prior knowledge one might have about the magnitude of the errors.

The prior distribution (A1) of  $\Sigma_k$  has the mean

$$\mathbf{E}(\boldsymbol{\Sigma}_k) = (\nu_k - n_k - 1)^{-1} \boldsymbol{W}_k,$$

where, as noted above,  $\nu_k$  is the parameter (degrees of freedom) that defines 471 the tightness (informativeness) of the prior and  $n_k$  is the length of the time 472 series  $\boldsymbol{y}_k$ . For the prior parameter  $\boldsymbol{W}_k$  we used a diagonal scale matrix 473  $\boldsymbol{W}_{k} = w_{k}\boldsymbol{I}_{n_{k}}$  such that  $E(\boldsymbol{\Sigma}_{k}) = \sigma_{k}^{2}\boldsymbol{I}_{n_{k}}$ , where  $\sigma_{k}$  is a fixed value. For 474 the time series Rapid and CR described in Sections 4.2 and 4.3 we used 475 the value  $\sigma_k = 0.75$ , an estimated root mean square error of prediction 476 (RMSEP) reported in *Miettinen at al.*, [2012]. For the time series NHem 477 described Section 4.4 we took  $\sigma_k = 0.15$ , a value estimated from the error 478 bars in Figure S5a of the Supplement to Mann et al. [2008]. Since now 479  $\sigma_k^2 \mathbf{I}_{n_k} = (\nu_k - n_k - 1)^{-1} w_k \mathbf{I}_{n_k}$ , we have  $w_k / \sigma_k^2 = \nu_k - n_k - 1$ . We took 480  $w_k = 5$  and  $w_k = 0.5$  for the first two and the third time series, respectively, 481 which corresponds to degrees of freedom  $\nu_k$  of 149, 219, and 264 for the 482 three time series. With these choices the prior 95% highest density intervals 483 for the diagonal elements of  $\Sigma_k$  were approximately [0.45, 1.15], [0.5, 1.15] 484

X - 28 GODTLIEBSEN ET AL.: SCALE-SPACE COMPARISON OF TIME SERIES and [0.11, 0.19] for the three time series and therefore wide enough to allow 485 also the data to have an effect on the posterior errors. It turned out that, 48F with very vague priors, the posterior errors of the first two time series were 487 smaller than the prior values which suggests that the values  $\sigma_k = 0.75$  used 488 probably is a bit too large for these temperature reconstructions and that 489 the credibility analysis of their features therefore tends to be somewhat 490 conservative. In contrast, the posterior errors of the third reconstruction 491 were very similar to their prior values. 492

We used the Gamma(1,1) prior for the parameter  $\kappa_k$  in (A2) in order not to smooth out the finest details in the reconstructions. However, after testing several different priors for  $\kappa_k$  we concluded that both the marginal posterior distribution of  $\kappa_k$  and the credibility maps produced were quite insensitive to a any particular reasonable prior choice.

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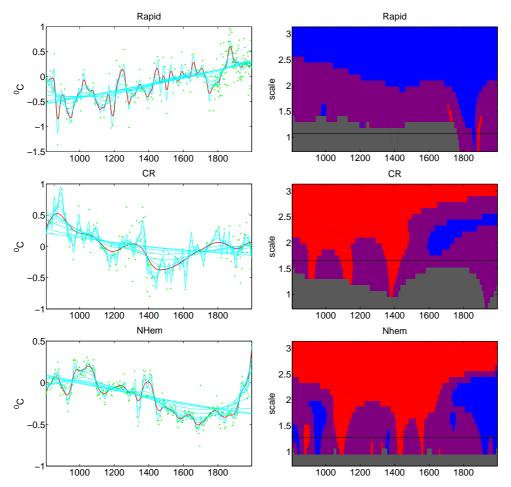
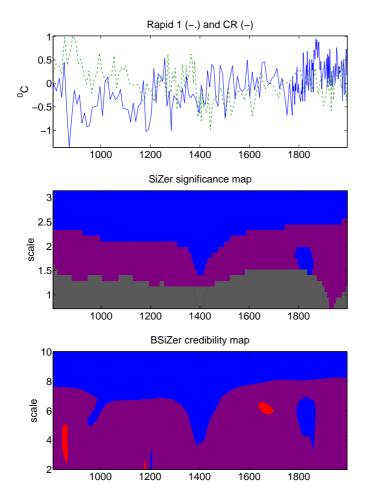


Figure 1. SiZer analyses of the three reconstructed temperature time series considered in the paper: Reykjanes Ridge SST (Rapid), Vøring Plateau SST (CR) and average Northern Hemisphere surface air temperature (NHem). Horizontal time scales indicate calendar years. On each row, the left panel displays a time series of reconstructed past temperatures (dots) together with a family of smooths. The right panel shows a SiZer significance map where, for a given time x and scale  $s = \log_{10}(h)$ , a pixel (x, s) is colored blue or red depending on whether the slope of the smooth of the true underlying temperature curve is significantly positive or negative, respectively. Purple indicates non-significance and pixels are colored gray if the data are too sparse to make any conclusions. The parallel distance between the dotted lines indicates the effective size of the smoothing kernel used for a particular scale, and hence gives an idea of the corresponding time-scale DRAFT February 2, 2012, 6:41pm DRAFT involved at that level of smoothing. The smoothing level corresponding to the red curve in the left panel is indicated by a horizontal line in the map.



**Figure 2.** Scale-space comparison of Reykjanes Ridge (Rapid) and Vøring Plateau SST (CR). Horizontal time scales indicate calendar years. Top panel: the two reconstructed temperature time series; Middle panel: SiZer significance analysis of the slope of the difference Rapid - CR. Blue (red) for each time and scale indicates whether the slope of the smooth of the true underlying temperature curve is significantly positive (negative). Purple indicates non-significance and pixels are colored gray if the data are too sparse to make any conclusions. Bottom panel: Bayesian credibility map of the slope of the difference Rapid - CR. The BSiZer credibility map is interpreted analogously with blue (red) color at a pixel indicating a credibly positive (negative) slope, respectively and purple indicating no credible change.

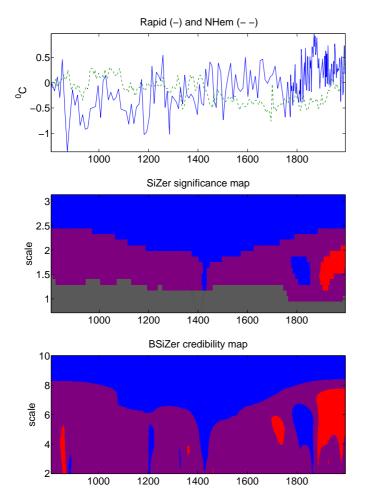
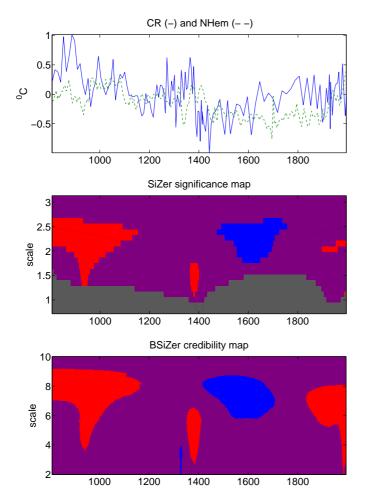


Figure 3. Scale-space comparison of Reykjanes Ridge SST (Rapid) and average Northern Hemisphere surface air temperature (NHem). Horizontal time scales indicate calendar years. Top panel: the two reconstructed temperature time series. Middle panel: SiZer significance analysis of the slope of the difference Rapid -NHem. Blue (red) for each time and scale indicates whether the slope of the smooth of the true underlying temperature curve is significantly positive (negative). Purple indicates non-significance and pixels are colored gray if the data are too sparse to make any conclusions. Bottom panel: Bayesian credibility map of the slope of the difference Rapid - NHem. The BSiZer credibility map is interpreted analogously with blue (red) color at a pixel indicating a credibly positive (negative) slope, respectively and purple indicating no credible change.



**Figure 4.** Scale-space comparison of Vøring Plateau SST (CR) and average Northern Hemisphere surface air temperature (NHem). Horizontal time scales indicate calendar years. Top panel: the two reconstructed temperature time series. Middle panel: SiZer significance analysis of the slope of the difference CR - NHem. Blue (red) for each time and scale indicates whether the slope of the smooth of the true underlying temperature curve is significantly positive (negative). Purple indicates non-significance and pixels are colored gray if the data are too sparse to make any conclusions. Bottom panel: Bayesian credibility map of the slope of the difference CR - NHem. The BSiZer credibility map is interpreted analogously with blue (red) color at a pixel indicating a credibly positive (negative) slope, respectively and purple indicating no credible change.