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climate4R: An R-based Open Framework for Reproducible Climate Data Access and Post-processing

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Abstract

Climate-driven sectoral applications commonly require different types of climate data (e.g. observations, reanalysis, climate change projections) from different providers. Data access, harmonization and post-processing (e.g. bias correction) are time-consuming error-prone tasks requiring different specialized software tools at each stage of the data workflow, thus hindering reproducibility. Here we introduce climate4R, an R-based climate services oriented framework tailored to the needs of the vulnerability and impact assessment community that integrates in the same computing environment harmonized data access, post-processing, visualization and a provenance metadata model for traceability and reproducibility of results. climate4R allows accessing local and remote (OPeNDAP) data sources, such as the Santander User Data Gateway (UDG), a THREDDS-based

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service including a wide catalogue of popular datasets (e.g. ERA-Interim, CORDEX, etc.). This provides a unique comprehensive open framework for end-to-end sectoral reproducible applications. All the packages, data and documentation for reproducing the experiments in this paper are available from http://www.meteo.unican.es/climate4R.

Keywords:

open science, climate indices, CMIP5, downscaling, climatic change, NetCDF-Java

1 1. Introduction

Climate data retrieval, harmonization and post-processing (e.g. bias correc-2 tion) are inherent tasks for climate vulnerability and impact assessment (VIA) 3 studies in a number of sectors such as agriculture, energy, hydrology, ecology, 4 health or wildfires among others (see, e.g. Casanueva et al., 2014; Ewert et al., 2015; Wang et al., 2017; Challinor et al., 2018; Walsh et al., 2018; Turco et al., 6 2018). Typically, these sector-specific applications require data for a reduced 7 number of surface variables from different sources (e.g. observations, reanalysis 8 and/or global and regional climate change projections), which can be directly ob-9 tained from different data providers and/or accessed through specialized data gate-10 ways such as the Earth System Grid Federation (ESGF; Williams et al., 2015). 11 However, the resulting formats, spatial and temporal scales and aggregations or 12 vocabularies (variable naming and units) are, as a rule, inhomogeneous across the 13 different data sources. Moreover, some common transformation/calibration and 14 post-processing steps are typically applied to raw model data before their use in 15 sectoral applications, including data collocation (e.g. regridding, temporal ag-

gregation, or subsetting) and bias adjustment or downscaling (e.g. local scaling, 17 quantile mapping, analogs or regression). In some cases, these steps are very tech-18 nical and require different specialized tools entailing multiple specific choices that 19 are often insufficiently documented in practical applications. As a result, obtain-20 ing and harmonizing climate data is typically an error-prone and time consuming 21 task, often preventing from an accurate replication of the research outcomes. The 22 difficulty of carrying out such processes remain as an important factor hampering 23 the full exploitation of available climate data to generate actionable information 24 leading to an "usability gap" (Lemos et al., 2012). 25

In order to bridge the usability gap, this paper presents a new R-based frame-26 work for climate studies, tailored to the specific needs of the VIA community, and 27 branded as climate4R. R (R Core Team, 2017) is nowadays a very popular com-28 puting environment with powerful statistical modeling tools and excellent support 29 for time series and spatial analysis, that has favoured its notable uptake by the cli-30 mate community. climate4R has been developed as a set of seamlessly integrated 31 packages designed to ease climate data access (loadeR), collocation and trans-32 formation (transformeR), bias correction and downscaling (downscaleR) and 33 visualization (visualizeR), including full documentation via wikis and guided 34 examples. Moreover, additional functionalities from existing external packages 35 have been bridged via specific climate4R wrapping packages so they can be 36 transparently used within the same framework. An example of external package 37 integration is climdex.pcic (Bronaugh, 2015), which implements the climate 38 extremes indices defined by the Expert Team on Climate Change Detection and 39 Indices (ETCCDI, Karl et al., 1999). Finally, a provenance metadata model for 40 traceability and reproducibility of results has been developed based on META-41

42 CLIP (METAdata for CLImate Products, http://www.metaclip.org), so full
43 metadata (including the source code) can be produced for all products generated
44 by climate4R.

climate4R is aimed at fostering research transparency and reproducibility, 45 issues of major concern in all experimental disciplines (see the special issue on 46 reliability and reproducibility of published research http://go.nature.com/ 47 huhbyr). For example, Baker (2016) recently reported that the work published in 48 Earth and Environment Science were mostly (over two-thirds) not reproducible. 49 As a result, there is growing concern among the scientific community about re-50 sults that cannot be reproduced. With this regard, one of the main objectives of 51 climate4R is to improve transparency and reproducibility of results. 52

Following with the above-mentioned study by Baker (2016), the main difficulties for research reproducibility identified include 1) access restrictions to raw input data and/or results, 2) methods or code unavailable and 3) incomplete metadata documentation of the particular workflow followed to obtain a climate product. In order to circumvent these problems, the following actions have been undertaken in climate4R:

1. Data sources: All the data needed for the experiments described in this 59 paper are publicly available at the Santander User Data Gateway (UDG, 60 http://www.meteo.unican.es/udg-wiki), a data service seamlessly in-61 tegrated with the climate4R framework, thus enabling a single entry point 62 for users to a wide variety of harmonized datasets, including global and re-63 gional climate projections from the Coupled Model Intercomparison Project 64 Phase 5 (CMIP5; Taylor et al., 2011a) and the COordinated Regional cli-65 mate Downscaling EXperiment (CORDEX; Giorgi and Gutowski, 2015) 66

respectively (see Sec. 3 for further details).

2. Source Code: All the R packages forming climate4R are publicly available
through the GitHub repository http://www.github.com/SantanderMetGroup.
Moreover, the full code to reproduce all the results presented in this work
(as well as extended examples) are included as auxiliary material as a paper
notebook https://github.com/SantanderMetGroup/notebooks.

3. Metadata: The R structures handled by climate4R are built upon the com-73 mon data model described in Sec. 2, and emphasis has been put on the 74 inclusion of all the necessary metadata for object description, including 75 spatiotemporal collocation details (dates/times, coordinates, geographical 76 projection, temporal resolution, etc.) and other relevant descriptors re-77 quired for their adequate characterization. Furthermore, climate4R is inte-78 grated within the METACLIP framework, envisaged to tackle the problem 79 of climate product provenance description. METACLIP is based on se-80 mantics exploiting web standard Resource Description Framework (RDF, 81 W3C, 2004), through the design of domain-specific extensions of stan-82 dard vocabularies (e.g., PROV-O; PROV Working Group, 2013; Moreau 83 et al., 2015) describing the workflow stages producing a climate product 84 (see http://www.metaclip.org for more details and worked examples, 85 including a full provenance description of Fig. 2a in this paper). 86

As a result, climate4R provides a unique framework for climate processing where most common tasks can be straightforwardly performed using a few lines of code, allowing end-to-end experimental reproducibility and facilitating the description (metadata) and documentation of the whole data flow. Although this paper focuses on the application of climate4R to climate change problems, this framework also allows to work with climate predictions, such as seasonal forecasts, an aspect that is separately described in Cofiño et al. (2018), with further
example research applications presented in Bedia et al. (2018a) and Frías et al.
(2018).

This article is structured as follows: Section 2 describes the core components 96 of climate4R. Sections 3 and 4 provide further aspects and details on the Data 97 Services Layer and the bias correction tools, respectively. Sections 5 and 6 present 98 two illustrative case studies. The first example describes the application to calcu-99 late and bias-correct future projections of a standard ETCCDI climate index (sum-100 mer days, http://etccdi.pacificclimate.org) for a Southern European do-101 main using locally stored CORDEX data. The second example illustrates an ex-102 tended case study accessing CORDEX data remotely from the Santander UDG. 103 Final conclusions are provided in Sec. 7. 104

105 2. The climate4R Framework

The climate4R data model is based on the Grid Feature Type (for gridded 106 data) and the Station Time Series Feature (for point data, e.g. stations or individ-107 ual gridbox values) implemented in the Unidata's Common Data Model version 4 108 (CDM¹). As such, the climate4R data access layer builds on Java to interpret 109 these CDM features (see Sec. 3) which are inherited by the R data/metadata 110 structures. The coordinate system for each object type includes, at least, the 111 time and position dimensions (latitude and longitude for grids and location for 112 point data). Besides the standard regular geographic coordinates, climate4R also 113

¹https://www.unidata.ucar.edu/software/thredds/current/netcdf-java/CDM/

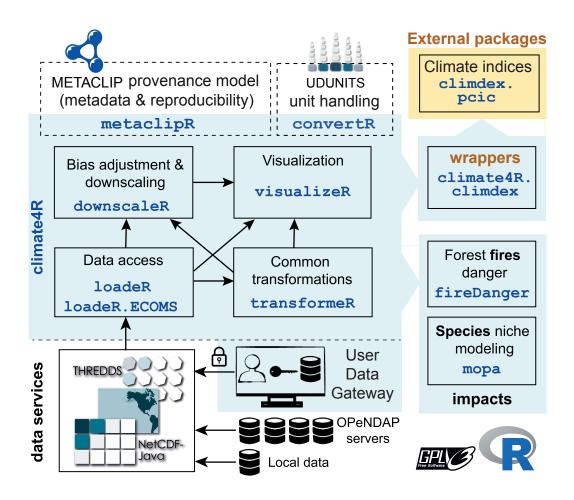


Figure 1: Schematic illustration of the climate4R framework consisting of three layers: (a) Data services building on NetCDF-Java and THREDDS in order to load local or remote (exposed via a THREDDS OPeNDAP service) data, and also datasets from the in-house Santander User Data Gateway (UDG); (b) The climate4R R bundle for data access and post-processing, formed by four core packages for data loading, transformation, downscaling (including bias correction) and visualization. These core packages are the basis for other sector-specific packages for impact analysis (e.g. forest fires, species distribution modelling, etc.) which further extend the climate4R capabilities. (c) External packages, which are connected to climate4R via specific wrapper packages. (d) Additional climate4R packages for extended functionality, including provenance meta-data model (based on METACLIP) or unit handling (based on UDUNITS). The arrows indicate the possible data flows and the blue shading differentiates the in-house developments. All components are distributed under GNU General Public License. The THREDDS, NetCDF-Java and UDUNITS logos are courtesy of UCAR/Unidata. The R logo is ©2016 The R Foundation. The RDF icon used by METACLIP is ©1994-2006 W3C.

handles rotated-pole and Lambert conformal conic projections used in CORDEX
 gridded datasets². Both grids and point datasets are transparently handled by all
 relevant climate4R functions.

Furthermore, the basic climate4R data structure includes additional dimen-117 sions, such as the *member*, which allows to work with ensembles. For instance, 118 this extra dimension is used when loading seasonal predictions using the loadeR. ECOMS 119 extension of the loadeR package (see Cofiño et al., 2018, for more details), tai-120 lored to the specific needs of the seasonal forecasting community. The member 121 dimension can be also used to construct multi-model ensembles. This poses sev-122 eral advantages from the user point of view, as next highlighted in case study 2 123 (Sec. 6). For instance, most of the climate4R operations (e.g. index calcula-124 tion and aggregation) are implemented to deal with grids containing the member 125 dimension and therefore, the necessary looping over several members is done be-126 hind the scenes. Furthermore, the use of members is also beneficial from the 127 computational point of view, since most relevant functions have the option to par-128 allelize across members through the optional argument parallel, thus providing 129 ease of use and computational efficiency. 130

A description of the core R packages forming the climate4R framework is next presented (see Fig. 1 for a schematic representation):

loadeR (Bedia et al., 2018b) is the central building-block of the climate4R
 bundle allowing to transparently access local and remote climate datasets
 (through the OPeNDAP service, see https://www.opendap.org) build ing on NetCDF-Java (see Sec. 3 for more details). Moreover, loadeR is

²http://is-enes-data.github.io/cordex_archive_specifications.pdf

the interface to the Santander User Data Gateway (UDG), a THREDDS-137 based (Unidata, 2006) service from the Santander Climate Data Ser-138 vice providing access to several climate datasets popular in impact stud-139 ies. A comprehensive description of functionalities of this package is 140 given in the loadeR's wiki (https://github.com/SantanderMetGroup/ 141 loadeR/wiki), as well as installation instructions and worked examples. 142 An extension of loadeR to work with climate predictions is also available 143 (loader.ECOMS), dealing with the initialization time (or lead time) selec-144 tion in a user-friendly way (see Cofiño et al., 2018). 145

transformeR (Bedia et al., 2018c) performs common data processing tasks
 such as regridding/interpolation, subsetting or spatio-temporal aggrega tion, among others. Unlike downscaleR, all the post-processing oper ations performed by transformeR do not necessarily entail a second
 reference observational dataset. Examples of application are available
 in the transformeR's wiki (https://github.com/SantanderMetGroup/
 transformeR/wiki).

downscaleR (Bedia et al., 2017) performs bias correction (see Sec. 4 for more
 details) and statistical downscaling. An introduction to the package and
 examples of application are available in the downscaleR's wiki (https:
 //github.com/SantanderMetGroup/downscaleR/wiki).

visualizeR (Frías et al., 2018) performs climate data visualization, implement ing basic visualization functionalities for gridded and point-based data, time
 series, and a set of advanced tools for forecast visualization in a form suit able to communicate the underlying uncertainty, such as tercile plots, bub-

ble plots, climagrams, reliability categories, etc. Examples and further func tionalities are detailed in the visualizeR's wiki (https://github.com/
 SantanderMetGroup/visualizeR).

Besides these core packages, climate4R extends its capabilities by integrating the functionalities of other external packages via auxiliary wrapping packages. For instance, the wrapper climate4R.climdex allows to transparently compute the 27 ETCCDI core indices implemented in the climdex.pcic R package³.

Furthermore, advanced unit checking and conversion can be achieved at any point during the data analysis via the climate4R package convertR (Bedia and Herrera, 2018), that exploits the Unidata's UDUNITS-2 software libraries (Unidata, 2017) —a widely used standard containing an extensive and user-extensible unit database in XML format— through its R binding package udunits2 (Hiebert, 2016). More information is available in the convertR GitHub repository (https://github.com/SantanderMetGroup/convertR).

In addition to the core and external climate4R packages, there are also spe-175 cific packages for some sectoral applications, such as fireDanger (Bedia et al., 176 2018a, implementing several popular fire-weather and drought indices) or mopa 177 (Iturbide et al., 2018, providing tools for species distribution modelling), which 178 are integrated within the climate4R framework. With this regard, the climate4R 179 data model has been conceived to minimize external dependencies and ease inter-180 operability, relying on basic R data structures. Conversion to other data formats 181 is straightforward for specific applications when needed, thus providing a flexible 182 framework for interacting with other packages of the R ecosystem according to 183

³http://github.com/pacificclimate/climdex.pcic

Dataset	Туре	Resolution(s)	Scenario	Members	Ref
WFDEI	Observations	0.50°	-	1	Weedon et al. (2014)
EWEMBI	Observations	0.50°	-	1	Lange (2016)
E-OBS	Observations	$0.25^{\circ} (0.22^{\circ} \text{ rot})$	-	1	Haylock M. R. et al. (2008)
Spain02	Observations	0.11° (0.1° rot)	-	1	Herrera et al. (2012, 2016)
ERA-Interim	Reanalysis	2°	-	1	Dee D. P. et al. (2011)
JRA55	Reanalysis	2°	-	1	Kobayashi et al. (2015)
CMIP5	Projections	2°	RCP4.5,8.5	10 GCMs	Taylor et al. (2011b)
EURO-CORDEX	Projections	0.44°, 0.11°	RCP4.5,8.5	12 RCMs	Jacob et al. (2014)
AFRICA-CORDEX	Projections	0.44°	RCP4.5,8.5	12 RCMs	Nikulin et al. (2012)

Table 1: Summary of the main public climate datasets available at the Santander User Data Gateway (UDG). For brevity, the datasets for seasonal forecasting are not included here (see Cofiño et al., 2018, and http://meteo.unican.es/ecoms-udg/catalog for details).

the specific user's needs. For instance, spatial data conversion to Spatial-class objects (Bivand et al., 2013) is internally done in visualizeR for specific geographical data representations, while mopa exploits the raster-class capabilities (Hijmans, 2017) to handle static climatological layers.

The following two sections provide further information on two aspects of climate4R of special relevance for better understanding the illustrative examples provided in this paper: the climate services layer and the available bias correction methods.

192 **3. Data Services Layer**

There is a number of R packages supporting read/write operations on NetCDF files, like ncdf, ncdf4 (Pierce, 2017), RNetCDF (Michna, 2014) and raster (Hijmans, 2017), all of them supporting both NetCDF-3 and 4 with the exception

of ncdf which only supports the older NetCDF-3 file format and has been there-196 fore removed from the R-CRAN repository since 2016. loadeR goes beyond 197 the file-oriented concept for data access, supporting reading (and writing) CDM 198 datasets, i.e. "collections" of NetCDF files, instead of individual files. Unlike 199 the file-based approach, the most immediate advantage from the user point of 200 view of using such collections is that one does not need to worry about a par-201 ticular directory tree structure or file naming schema when the required data is 202 split into several files (usually due to size constraints), and only one single URL 203 pointing to the dataset need to be used, as if all the data was contained in a single 204 "file". loadeR allows for a direct creation of such CDM datasets from R (function 205 makeAggregatedDataset), so multiple CDM files can be conveniently combined 206 ("aggregated") along the selected dimension(s), a process that is fully automatized 207 for the most usual cases that users typically face after raw data retrieval from ex-208 ternal repositories/servers. This entails for instance joining different files of the 209 same variable along the specified dimensions (e.g., joining files along time) and/or 210 performing unions of different variables stored in separate files to obtain a single 211 multi-variable dataset. However, loadeR is also able to read from single files if 212 preferred by the user, following exactly the same procedure as reading from CDM 213 datasets. 214

By exploiting the capabilities of the NetCDF-Java libraries built upon Unidata's CDM (Sec. 2), loadeR also allows for an efficient access to remote datasets via OPeNDAP, providing users a transparent access to the data regardless of whether these are stored locally or remotely. This is internally achieved through the r Java package (Urbanek, 2016) that provides a low-level interface between R and the Java virtual machine. In addition, not only NetCDF, but also a variety of other geoscientific data formats (HDF, GRIB, etc.) can be aggregated to
produce CDM datasets via the NetCDF Markup Language (NcML) and accessed
by loadeR using identical code. NcML is an XML dialect that allows not only
creating CDM datasets, but also to modify (rename, add, delete and/or restructure)
the data and metadata of the original NetCDF files and/or CDM datasets, without
the need of modifying the original files.

227 3.1. The Santander User Data Gateway

Besides local and remote OPeNDAP datasets, climate4R is transparently 228 connected to the User Data Gateway (UDG), from the Santander Climate 229 Data Service hosted by University of Cantabria (http://meteo.unican.es/ 230 udg-wiki) consisting of two main components: (1) A THREDDS Data Server 231 (TDS) and (2) the THREDDS Access Portal (TAP), which provide standard ser-232 vices for data access (e.g. OPeNDAP or the NetCDF Subset Service -NCSS-) and 233 user management and authentication (based on data policies associated with vir-234 tual datasets), respectively. The UDG provides harmonized access to a variety of 235 common datasets typically used in sectoral applications, including state-of-the-art 236 global and regional climate projections such as those from CMIP5 (Taylor et al., 237 2011a) and CORDEX (Giorgi and Gutowski, 2015). Thus, the UDG represents 238 a one-stop-service for climate data access where users can efficiently retrieve the 239 subsets best suited to their particular research aims (for particular regions, periods 240 and/or ensemble members) and where dataset access is controlled through a fine-241 grained authorization scheme depending on the different data policies (there is a 242 wide variety of datasets of public access through the PUBLIC role, see Table 1). 243

4. Bias Correction Methods

The R package downscaleR implements several statistical downscaling 245 (analogs, generalized linear regression, neural networks, etc.) and bias correc-246 tion (scaling, parametric and empirical quantile mapping, etc.) methods, some of 247 which have been already used and tested in the VALUE initiative (Gutiérrez et al., 248 2018). In this paper we focus on bias correction methods, which adjust model out-249 puts, e.g. maximum temperature in this paper, using as reference the correspond-250 ing local observations (either point-wise stations or an interpolated grid, E-OBS 251 in this paper). Bias correction methods are trained over a representative historical 252 period (typically 30 years), and then applied to correct model outputs for a test 253 (or future) period. Due to their simplicity and straightforward application, these 254 methods have become very popular during the last decade and have been used in 255 numerous recent papers covering different forecast temporal horizons. However, 256 it is important to understand their assumptions and limitations in order to avoid 257 the misuse of these techniques (see, e.g., Maraun et al., 2017; Manzanas et al., 258 2017b). 259

The biasCorrection function is the workhorse to apply several standard bias correction techniques, ranging from the simplest local-scaling to more sophisticated parametric or empirical quantile-quantile mapping approaches. Next, we provide a brief description of the two bias correction methods that are used in this work (for further information on all available methods, the reader is referred to the downscaleR's wiki):

Local-scaling: This method is specified by the argument method = "scaling". It consists in scaling the predictions with an additive (scaling.type = "additive") or multiplicative (scaling.type = "multiplicative")

269	factor, which is obtained as the difference/ratio between the predicted and
270	the observed mean in the train period. The additive version is preferable for
271	unbounded variables (e.g. temperature) and the multiplicative is typically
272	used with variables with lower bound = 0 (e.g. precipitation or wind speed).

Empirical quantile mapping (EQM): This method is applied using the argument 273 method = "eqm". The EQM method does not make any assumption about 274 the statistical distribution of the variable and consists in calibrating the 275 empirical predicted Cumulative Distribution Function (CDF) by adjusting 276 the model quantiles towards the observed ones (Déqué, 2007). The op-277 tional argument n.quantiles allows to specify the number of quantiles 278 to be adjusted (by default, percentiles are used for the correction). More-279 over, different extrapolation alternatives can be selected via the parameter 280 extrapolation. For the case of precipitation, the frequency adaptation 281 proposed by Themeßl et al. (2012) is applied by default when the predicted 282 frequency of dry days is larger than the observed one. A precise description 283 of the EQM method, as used in this paper, is provided in Appendix A of 284 Gutiérrez et al. (2018). 285

Additionally, in order to tackle the issue of seasonality —and also model drift in seasonal forecasting (see, e.g., Manzanas, 2016),— the optional argument window allows to specify the center and width of a moving time window (calendar days) that can be used for independently correcting consecutive periods (e.g. months or seasons), instead of the total available period at once. Moreover, biasCorrection deals with the ensemble dimension, allowing to separately correct each member (join.members = FALSE, e.g. for multi-model ensembles in climate change applications), or to use the joint ensemble distribution as reference (join.members = TRUE, e.g. for different members of a seasonal forecast
system, that are by definition statistically indistinguishable).

Furthermore, all bias correction methods can be applied in cross-validation mode with the argument cross.val (see the downscaleR's wiki for examples of application), which allows for leave-one-out ("loo") and k-fold ("kfold") crossvalidation schemes (see, e.g., Maraun et al., 2015; Manzanas et al., 2017a).

In order to promote a collaborative development of the bias correction meth-300 ods, these are implemented as atomic functions that receive vectors as input (ob-301 servations, predictions and, for methods requiring calendar information, the corre-302 sponding dates), so contributors do not need to worry about the particularities and 303 complexities of internal metadata handling. biasCorrection recursively applies 304 these methods to the N-dimensional arrays of the climate4R data model, accord-305 ing to the different optional arguments provided (e.g. cross-validation method, 306 parallel computing options, window size, etc.) and performing metadata update 307 as required. 308

5. Example 1: Climate Indices from CORDEX Projections

The main functionalities of climate4R are showcased describing the complete workflow needed to compute and bias correct an ETCCDI climate index (implemented in the R package climdex.pcic, Bronaugh, 2015, see also http:// etccdi.pacificclimate.org/list_27_indices.shtml) from locally stored EURO-CORDEX Regional Climate Model (RCM) data (Jacob et al., 2014). In particular, in this example we consider the projections of summer days (SU) defined as the number of days with maximum temperature > $25^{\circ}C$ — for a single model over a Mediterranean domain. The second case study (Sec. 6) will further
expand on this example illustrating a more comprehensive analysis that builds a
multi-model ensemble from EURO-CORDEX data, retrieved remotely from the
Santander UDG.

In the following, some code is interwoven within the text in order to illustrate the main package functionalities (the lines of code are identified by the R prompt symbol ">"). As a first step, the climate4R packages can be installed⁴ from the GitHub repository using the devtools package:

> library(devtools)

```
> install_github(c("SantanderMetGroup/loadeR",
```

"SantanderMetGroup/loadeR.java",
"SantanderMetGroup/transformeR",
"SantanderMetGroup/visualizeR",
"SantanderMetGroup/downscaleR",
"SantanderMetGroup/climate4R.climdex")

³²⁵ 5.1. Loading, collocating and harmonizing data

In this section, we show the climate4R data access capabilities (including on-the-fly temporal aggregation and filtering), in order to directly load monthly summer days (SU) from the original maximum daily temperature data. However, only a reduced set of indices can be directly obtained in this way. Thus, in Sec. 5.3 we revisit this example working with the original daily data. This leads to a

⁴loadeR depends on package rJava, which might present installation problems as reported by some users. See the related loadeR's Wiki section for help and installation recommendations: https://github.com/SantanderMetGroup/loadeR/wiki/Installation

more general approach where a variety of indices can be computed using, e.g., the climdex.pcic package implementing the 27 ETCCDI core indices (which include SU).

First, we describe the use of loadeR to load data subsets from the two datasets used in this example: (1) remote E-OBS gridded observations from the E-OBS OPeNDAP server⁵, and (2) locally stored regional climate projections from a particular EURO-CORDEX RCM (for both the historical and the RCP8.5 scenarios) previously downloaded from ESGF —see Appendix A—.

The following call to the function loadGridData retrieves the E-OBS maxi-339 mum temperature (var = "tx") field of the full year (season = 1:12), from a 340 single remote NetCDF file (dataset = eobs_url), considering a Mediterranean 341 spatial domain (lonLim = c(-10, 20), latLim = c(35, 46)) for a historical 342 period (years = 1971:2000). In order to compute the SU index on-the-fly at a 343 monthly scale, optional arguments are used both for data filtering (condition = 344 "GT", threshold = 25, to indicate the binary filtering "strictly greater than 25") 345 and aggregation (aggr.m = "sum", to indicate the monthly aggregation func-346 tion). 347

> library(loadeR)

⁵The E-OBS dataset URL is not persistent, being updated with each new version of the dataset. Please check the ECA&D site for the current E-OBS version and its corresponding active OPeN-DAP URL at http://opendap.knmi.nl/knmi/thredds/e-obs/e-obs-catalog.html

```
season = 1:12,
years = 1971:2000,
lonLim = c(-10, 20),
latLim = c(35, 46),
aggr.m = "sum",
condition = "GT",
threshold = 25)
```

Data transformation (e.g. regridding or additional temporal aggregation), is facilitated by the various functions of the transformeR package, and visualization capabilities are provided by the visualizeR package. For instance, the following commands perform annual aggregation and plot the climatological map of the resulting annual SU index:

```
> library(transformeR); library(visualizeR)
```

- > SU <- aggregateGrid(SU, aggr.y = list(FUN = "sum"))</pre>
- > # Generates Figure 2a:
- > spatialPlot(climatology(SU))

EURO-CORDEX regional climate change projections from the RCA RCM driven by the EC-EARTH GCM— can be loaded in a similar way. The NetCDF files of these simulations were downloaded from ESGF and stored locally (as detailed in Appendix A):

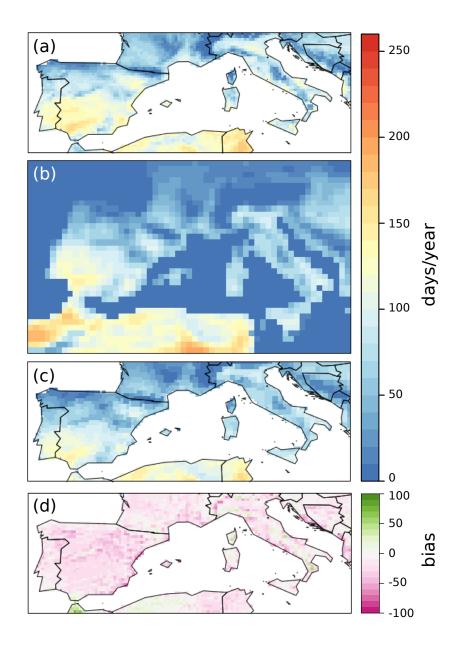


Figure 2: Annual climatology of Southern Europe summer days (ETCCDI SU index) for the reference period 1971-2000 according to: (a) 0.22° E-OBS gridded observations dataset, (b) 0.44° RCA regional climate model (driven by EC-EARTH GCM, historical scenario), (c) same as (b), but after regridding onto the regular E-OBS grid and (d) RCM bias (days/year) w.r.t. E-OBS.

- > dir <- "/myDirectoryHistoricalScenario/"</pre>
- > list.files(dir, recursive = TRUE)
- # [1] "tasmax_EUR-44_EC_hist_SMHI-RCA4_2006-2010.nc"
- # [2] "tasmax_EUR-44_EC_hist_SMHI-RCA4_2011-2015.nc"

```
# [3] "tasmax_EUR-44_EC_hist_SMHI-RCA4_2016-2020.nc"
```

. . .

Note that, in this case, five-year periods are stored in separate files. As ex-357 plained in Sec. 2, one key strength of loadeR is that, in addition to single 358 files —which can be directly loaded with loadGridData as in the previous E-359 OBS case-, it can transparently work with collections of files (catalogs) with 360 a single access point (given by a NcML file; see Sec. 3 for more details). 361 This greatly facilitates data access, separating the logical structure of files from 362 the way these are accessed. The following code shows the use of functions 363 makeAggregatedDataset and dataInventory to write a catalog including the 364 information contained in the files within a particular directory (in this case 19 files 365 containing maximum temperature data for the period 2006-2100), and to display 366 an overview of the dataset from the resulting NcML file (CDX_hist.ncml in this 367 example): 368

- # \$ Description: chr "Daily Maximum Near-Surf...

\$ DataType : chr "float" # \$ Units : chr "K" # \$ Dimensions :List of 3 # ..\$ time:List of 4 #\$ Type # : chr "Time" #\$ TimeStep : chr "1.0 days"\$ Units : chr "days since 1949-12-0... # #\$ Date_range: chr "2006-01-01T12:00:00Z... # ..\$ lat :List of 3 #\$ Type : chr "GeoY" #\$ Units : chr "degrees"\$ Values: num [1:103] -23.2 -22.8 -22.3... # # ..\$ lon :List of 3\$ Type : chr "GeoX" #\$ Units : chr "degrees" # #\$ Values: num [1:106] -28.2 -27.8 -27.3...

Note that the units of this dataset are given in Kelvin (*K*). Therefore, harmonization with E-OBS units (*degC*) is required. This can be done using the function 'udConvertGrid' from package 'convertR' (see Sec. 2) after data load, or directly on load using the harmonization capability implemented in climate4R through the definition of a standard vocabulary (complying with the UDUNITS standards) and the possibility to create raw-to-standard dictionaries for particular datasets. The climate4R standard vocabulary is displayed by function C4R.vocabulary:

> C4R.vocabulary()

identifier standard_name units
...

17 tas 2-meter air temperature degC # 18 maximum 2-m air temperature degC tasmax minimum 2-m air temperature # 19 tasmin degC # 21 total precipitation amount pr mm . . .

A dictionary is a text file including simple unit conversion parameters (offset and 376 scale) as well as temporal characterization attributes (further information can be 377 found in the wiki https://github.com/SantanderMetGroup/loadeR/wiki/ 378 Harmonization). The construction of a dictionary for a dataset should be care-379 fully performed (with the help of dataInventory) and may require detailed in-380 formation from the data owner (e.g. temporal attributes). The dictionary file is 381 usually saved locally —for instance together with the dataset— for its repeated 382 usage (further instructions on dictionary usage are given in the loadGridData 383 help menu). For better reproducibility, in the following code chunk a dictionary 384 for the CORDEX RCM dataset is created on-the-fly as a temporary file to con-385 vert the raw maximum temperature units (K) to the stand ones (degC). Note that 386 the code for this variable is the same (tasmax) in the CORDEX and standard 387 vocabularies, as specified in the dictionary with short_name and identifier, 388 respectively. 389

```
> dic <- tempfile(pattern = "cordex", fileext = ".dic")
> writeLines(c(
    "identifier,short_name,time_step,lower_time_bound,
        upper_time_bound, cell_method,offset,scale,
```

deaccum, derived, interface",

"tasmax,tasmax,24h,0,24,max,-273.15,1,0,0,"), dic)

The dictionary can be passed to loadGridData by the optional argument dictionary = dic; otherwise the original data would be loaded in its original units:

```
> SUh <- loadGridData(dataset = "CDX_hist.ncml",</pre>
```

```
var = "tasmax",
season = 1:12,
lonLim = c(-10, 20),
latLim = c(35, 46),
years = 1971:2000,
aggr.m = "sum",
threshold = 25,
condition = "GT",
dictionary = dic)
> SUh <- aggregateGrid(SUh, aggr.y = list(FUN = "sum"))</pre>
```

```
> # Generates Fig 2b:
```

```
> spatialPlot(climatology(SUh))
```

Note that the CORDEX RCM data is provided in rotated coordinates (Figure 2b) and therefore, regridding is needed in order to compare the results with E-OBS, so basic arithmetic operations can be applied (e.g. 'difference' to obtain the bias). This can be achieved using the interpGrid function. It uses the nearest gridbox by default, but additionally, two different bilinear interpolation implementations are available. In this example, the rotated coordinates of the RCM are interpolated onto the regular E-OBS grid:

```
> SUh <- interpGrid(SUh, getGrid(SU))</pre>
```

> # Generates Fig 2c:

- > spatialPlot(climatology(SUh))
- > bias <- gridArithmetics(SUh, SU, operator = "-")</pre>
- > # Generates Fig 2d:
- > spatialPlot(climatology(bias))

Similar data access and regridding operations are followed to load the projections of RCP 8.5 scenario (e.g. for the period 2071-2100), obtaining the future summer days (SUf, Figure 3a) and the climate change signal (delta, Figure 3b), as the difference with the historical signal (see the auxiliary notebook for the full code).

Note that the results obtained from CORDEX are affected by systematic biases —see Fig. 2d,— which prevent their direct use in most impact studies. Therefore, these results are typically post-processed in order to adjust the bias using *bias correction* techniques.

409 5.2. Post-processing: Bias Correction

The function biasCorrection of package downscaleR allows applying a 410 number of standard bias correction techniques within the climate4R framework 411 (see Sec. 4). In particular, when dealing with monthly data (as in the present 412 example), the common bias correction technique is the (additive and/or multi-413 plicative) local scaling method (Sec. 4). The projections of future summer days 414 (newdata = SUf) are corrected using the method calibrated using the historical 415 model as training data ("predictor", x = SUh) and the observed reference data 416 ("predictand", y = SU): 417

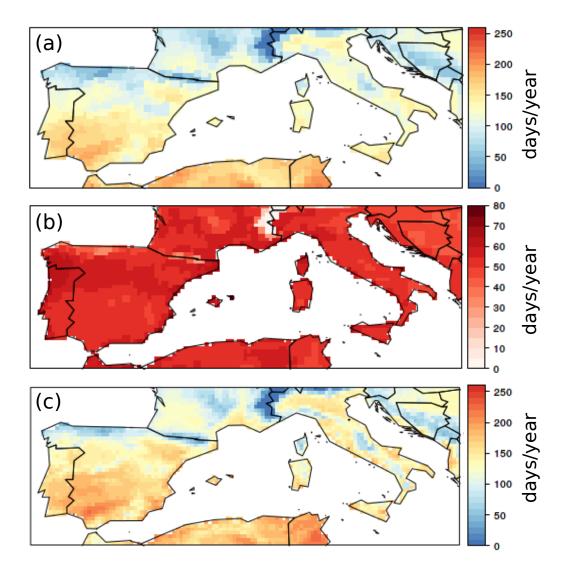


Figure 3: Climatology of Southern Europe annual SU (summer days) for the future period 2071-2100: (a) RCA (EC-EARTH driven, RCP8.5 scenario) RCM, (b) climate change signal (delta) w.r.t. the historical 1971-2000 RCA value —Figure 2c—, (c) bias corrected (additive scaling, based on E-OBS) results.

> spatialPlot(climatology(SUf.bc))

The function temporalPlot displays temporal series for several datasets and periods on the same plot. temporalPlot is based on the powerful lattice package (Sarkar, 2008) and therefore, fine-tuning plotting parameters can be passed through the argument xyplot.custom (see the auxiliary notebook). In this case, we are plotting the series of a single gridbox, the one closest to Zaragoza (with coordinates latLim = 41.64, lonLim = -0.89).

```
> # Generates Fig. 4:
```

> temporalPlot("E-OBS" = SU,

```
"CDX_hist" = SUh,
"CDX_rcp85" = SUf,
"CDX_rcp85_corrected" = SUf.bc,
latLim = 41.64, lonLim = -0.89,
cols = c("black", "red", "red", "blue"))
```

The resulting figure (Fig. 4) shows the inter-annual SU time series for the selected gridbox point (Zaragoza), highlighting the large model bias (red) *w.r.t.* the observations (black) in the historical period. This figure also shows how bias
correction compensates for this bias when applied to the future period (red *vs* blue
for 2071-2100).

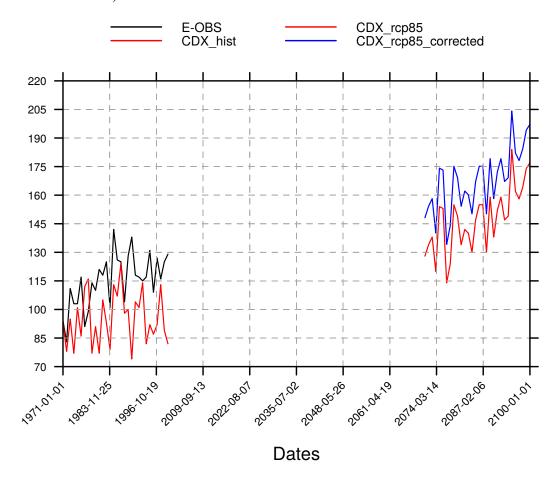


Figure 4: Annual summer days time series for a single gridbox (the one closest to Zaragoza, in the Ebro valley, Spain) for the observations (E-OBS) and the projection (original and bias corrected) in the historical and future periods.

429 5.3. Working with daily data

Loading aggregated data (monthly in the example above) is a useful feature allowing for an efficient use of memory. However, as we already mentioned, only a reduced set of indices can be directly obtained in this way. Therefore, in this section we revisit this example considering a more general approach using daily data and the climate4R.climdex package for index calculation (a wrapper of climdex.pcic, implementing the 27 ETCCDI core indices).

The data loading process for E-OBS (TX) and the historical (TXh) and future (TXf) RCM data is similar to the previous cases, but omitting the aggregation and filtering options. For instance the historical period can be loaded by:

```
> TXh <- loadGridData(dataset = "CDX_hist.ncml",</pre>
```

```
var = "tasmax",
season = 1:12,
lonLim = c(-10, 20),
latLim = c(35, 46),
years = 1971:2000,
dictionary = dic)
```

In this case, it is possible to apply bias correction methods better suited for daily data than local scaling, before calculating the index. For instance, in the example below we use empirical quantile mapping (method = "eqm") with a moving window of 30 days to correct each 7-day time interval (see Sec. 4 for EQM method description and argument explanation):

```
newdata = TXf,
method = "eqm",
window = c(30, 7),
extrapolation = "constant")
> SUf <- climdexGrid(tx = TXf, index.code = "SU")
> SUf.bc <- climdexGrid(tx = TXf.bc, index.code = "SU")
> # Generates Fig. 5:
> spatialPlot(climatology(SUf.bc))
```

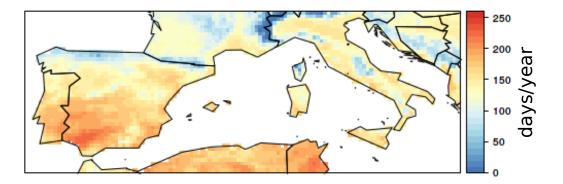


Figure 5: As Figure 3c, but for the index computed from bias corrected (empirical quantile mapping) daily maximum temperature data.

The resulting bias-corrected index (Fig. 5) is only slightly different to the one computed with monthly data in the previous section (Figures 3c). Therefore, both bias correction approaches lead to similar results in this case (see Casanueva et al., 2018, for further discussion on direct vs component-wise bias correction). More comprehensive experiments considering different indices and spanning more bias correction techniques could be easily undertaken using the functions here shown (more examples are provided in the auxiliary notebook).

6. Example 2: Working with remote data from the UDG

The Santander User Data Gateway (UDG) is a data service providing harmonized remote access to a number of popular datasets in climate studies (a summary is given in Table 1) which is seamlessly integrated with climate4R (see Sec. 3.1). In this section we extend the analysis performed in the previous example building a multi-model ensemble of CORDEX projections for the SU index and assessing the resulting uncertainty.

The UDG service requires (free) registration to accept the data policies of the different data providers (http://www.meteo.unican.es/udg-wiki). Prior to data access, authentication with valid UDG credentials is required for the current R session in order to access the UDG. Once a valid user name and password have been issued, the authentication can be done in one step within the R session using the loginUDG function from loadeR:

- > library(loadeR)
- > loginUDG("userUDG", "pswrdUDG")
- # Setting credentials...

Success!

- # Go to <http://www.meteo.unican.es/udg-tap/home>
- # for details on your authorized groups and datasets

It must be noted that it is insecure and in general not advisable to pass the user name and password in plain text within the scripts, although here it is shown this way for illustration purposes. Mechanisms exist in R to ensure a secure transfer of personal data and to avoid revealing personal passwords when sharing code (see e.g. https://cran.r-project.org/web/packages/httr/vignettes/ secrets.html).

The function UDG.datasets() prints a list of the UDG datasets readily avail-470 able from climate4R showing the name, type (i.e. observation, reanalysis or 471 projection) and URL. The harmonization capability for all these datasets is given 472 by the predefined dictionaries included in loadeR. The use of these internal dic-473 tionaries is activated by default when using the name of the target dataset as an 474 entry for the argument dataset in loadGridData, instead of the full URL. In 475 the following example, we use this option to load CORDEX data, thus, unlike in 476 Example 1 (Sec. 5), there is no need for posterior conversion to the climate4R 477 standard naming and units. 478

For a lighter computational and memory demand, here we restrict the analysis to the Iberian Peninsula (arbitrary spatial domains can be indicated by changing the lonLim and latLim argument values) and use the 0.44° regular grid (note that the 0.11° simulations are also available at UDG). When listing the available datasets, pattern matching can be used to locate datasets with particular characteristics through the optional argument pattern:

> mod <- UDG.datasets(pattern = "CORDEX-EUR44.*hist")</pre>

> mod\$name

- #[1] CORDEX-EUR44_ICHEC-EC-EARTH_r12i1p1_RCA4_v1_hist
- #[2] CORDEX-EUR44_CERFACS-CNRM-CM5_r1i1p1_RCA4_v1_hist
- #[3] CORDEX-EUR44_ICHEC-EC-EARTH_r1i1p1_RACMO22E_v1_hist
- #[4] CORDEX-EUR44_ICHEC-EC-EARTH_r3i1p1_HIRHAM5_v1_hist
- #[5] CORDEX-EUR44_IPSL-CM5A-MR_r1i1p1_RCA4_v1_hist
- #[6] CORDEX-EUR44_MOHC-HadGEM2-ES_r1i1p1_RCA4_v1_hist

• • •

A multi-model ensemble (e.g. the first 6 models in this example) can be ac-

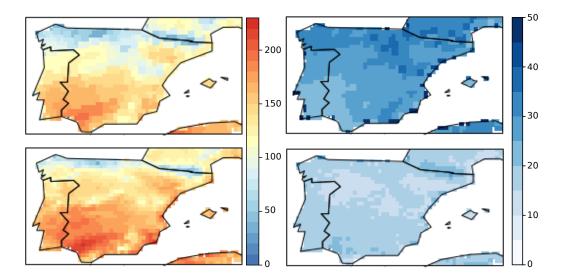


Figure 6: Summer days in Iberia for the future period 2071-2100 computed from the original RCM daily maximum temperature data (above), and daily maximum temperature bias corrected data using E-OBS (below). The left column shows the ensemble mean, whereas the right column shows the ensemble standard deviation (uncertainty).

⁴⁸⁶ cessed using a loop on the target datasets (lapply in this example):

⁴⁸⁷ The six model outputs are next regridded onto the E-OBS grid (the step is

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detailed in the auxiliary notebook) and the multi-model ensemble is constructed with function bindGrid.

```
> TXh.ens <- bindGrid(TXh.list, dimension = "member")
> str(TXh.ens)
```

Note that the new ensemble data structure contains the additional dimension member, that includes the six members composing the multi-model, as described in Sec. 2. The same process is followed to obtain the RCP 8.5 future ensemble (TXf . ens, see the auxiliary notebook). As a result of arranging all the ensemble members within the same structure, SU index calculation can be performed for the whole ensemble in a single line of code. Additionally, the member dimension can be directly aggregated to calculate the ensemble mean and deviation (Fig. 6(top)).

Bias correction (empirical quantile mapping in this example, method = "eqm") is performed similarly, with the possibility to include further arguments (join.members) to control how the members are treated within the bias correction step. By default, each member is corrected separately: TXf.ens.bc <- biasCorrection(y = TX,</pre>

x = TXh.ens, newdata = TXf.ens, window = c(30, 7), method = "eqm")

The SU ensemble mean projection and the corresponding uncertainty (as char-501 acterized by the standard deviation of the multi-model) can be directly obtained 502 for the bias-corrected data by repeating the above code producing the top panels 503 of Fig. 6, but using the bias-corrected ensemble TXf.ens.bc instead of TXf.ens, 504 as shown in the two bottom panels of Fig. 6. Finally, the resulting time series for 505 the target location (Zaragoza) are shown in Fig. 7, where the uncertainty of the 506 ensemble is depicted by shaded areas representing the multi-model range (see the 507 auxiliary notebook for the full code). 508

These results show that a large reduction of the uncertainty is achieved for SU 509 projections after correcting the bias of the original maximum temperature data, 510 highlighting the need for bias-corrected data prior to index calculation. As SU 511 is based on an absolute threshold $(25^{\circ}C)$, the biases of the different ensemble 512 members largely affect the threshold exceedances, as shown in Figure 8 (see the 513 code in the auxiliary notebook). However, these results might be different for 514 relative (e.g. percentile-based) threshold indices that do not make use of absolute 515 values. Unlike SU, an example for the ETCCDI index CDD (consecutive dry 516 days) is provided in the auxiliary notebook, yielding no significant uncertainty 517 reduction after bias correction. 518

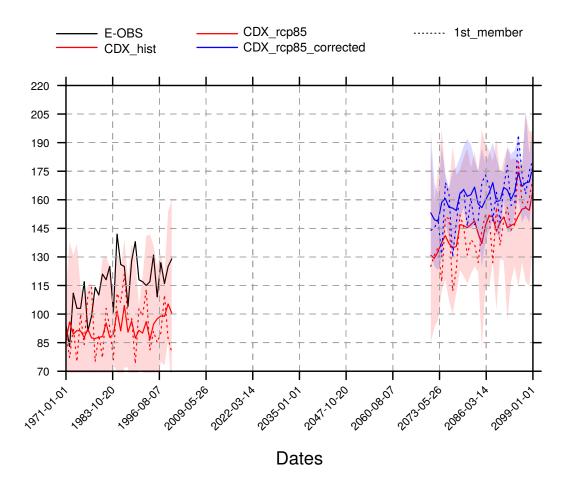


Figure 7: Annual summer days time series for a single gridbox (the one closest to Zaragoza, in the Ebro valley, Spain) computed from (red) the original RCM daily maximum temperature data, and (blue) daily maximum temperature bias corrected data using E-OBS (black). When it comes to CORDEX data, continuous lines correspond to the ensemble mean and the shadowed area to the range (uncertainty). Dashed lines correspond to the 1st member of the ensemble, the same as the one used in Sec. 5 (see Fig. 4).

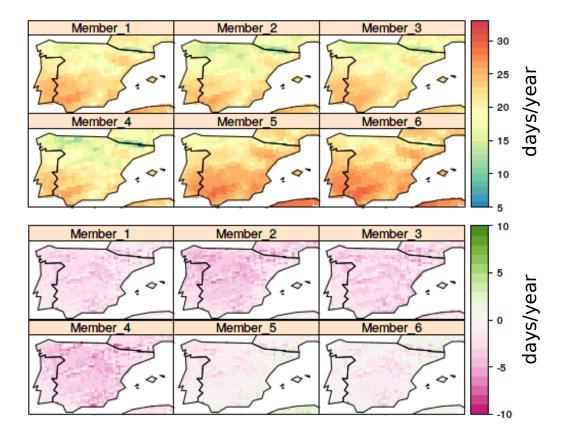


Figure 8: (Top) Maximum temperature in Iberia for the future period 2071-2100 (RCP8.5 scenario) for six CORDEX models. (Bottom) Bias of the RCMs (historical scenario w.r.t. E-OBS for the period 1971-2000).

519 7. Conclusions

This paper introduces the climate4R framework for accessing and postprocessing climate data within the R computing environment, and describes its main components (data services, core packages and external packages) and functionalities, including two practical illustrative case studies that showcase its main functionalities. The first example describes the application to calculate and bias-

correct future projections of a standard ETCCDI climate index (summer days) 525 for a Southern European domain from locally stored CORDEX data. The sec-526 ond example illustrates an extended case study using remote data (from the San-527 tander UDG) to construct an ensemble of future regional climate projections 528 for different climate indices and to analyze the sensitivity of the results (in-529 cluding the potential reduction of uncertainty after bias correction). Moreover, 530 a companion notebook allows the full reproducibility of the examples (https: 531 //github.com/SantanderMetGroup/notebooks). 532

Throughout these examples it has been shown how the different tools avail-533 able in the climate4R framework allow for: 1) an easy harmonized access 534 of user-defined slices from complex datasets —either locally or remotely via 535 OPeNDAP—, 2) flexible data handling, 3) quick and powerful visualization ca-536 pabilities and 4) straightforward application of a wide range of bias correction 537 methods, providing an intuitive interface for undertaking many different climate 538 data operations usually required by the climate VIA community, and easing the 539 performance of complex research experiments and their end-to-end reproducibil-540 ity. 541

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553 Software and data availability

554	All data used in this paper is publicly available (details are provided in Sec-
555	tions 3, 5 and 6).
556	climate4R packages used in this paper are the following:
557	'loadeR' (version 1.4.6)
558	'transformeR' (version 1.4.4)
559	'downscaleR' (version 3.0.3)
560	'visualizeR' (version 1.2.2)
561	'climate4R.climdex' (version 0.1.4)
562	
563	Developers in alphabetical order: J. Baño-Medina, J. Bedia, E. Cimadevilla,
563 • 564	Developers in alphabetical order: J. Baño-Medina, J. Bedia, E. Cimadevilla, A.S. Cofiño, J. Fernández, M. D. Frías, J. M. Gutiérrez, S. Herrera, M.
564 565	A.S. Cofiño, J. Fernández, M. D. Frías, J. M. Gutiérrez, S. Herrera, M.
564 565 566	A.S. Cofiño, J. Fernández, M. D. Frías, J. M. Gutiérrez, S. Herrera, M. Iturbide, R. Manzanas, D. San-Martín.
564 565 566 567	A.S. Cofiño, J. Fernández, M. D. Frías, J. M. Gutiérrez, S. Herrera, M. Iturbide, R. Manzanas, D. San-Martín.Website: https://github.com/SantanderMetGroup.

570	•	Installation	code:

571	<pre>> library(devtools)</pre>
572	<pre>> install_github(c(</pre>
573	"SantanderMetGroup/loadeR.java",
574	"SantanderMetGroup/loadeR",
575	"SantanderMetGroup/transformeR",
576	"SantanderMetGroup/visualizeR",
577	"SantanderMetGroup/downscaleR",
578	"SantanderMetGroup/climate4R.climdex")

579 Licensing

This software is made freely available under the terms and conditions of the GNU General Public License Version 3.

⁵⁸² Appendix A. Downloading data through ESGF

Earth System Grid Federation (ESGF, https://esgf.llnl.gov/mission. 583 html) is a worldwide distributed infrastructure for the management and access 584 to the climate data produced in different international initiatives as the differ-585 ent phases of the Coupled Model Intercomparison Project (CMIP) or the Co-586 ordinated Regional Climate Downscaling Experiment (CORDEX). ESGF nodes 587 (https://esgf.llnl.gov/nodes.html) are the access point to search, ex-588 plore and download this large amount of data independently on the server in 589 which they are located. In spite of the common access, in order to down-590 load the data several previous steps should be made, introducing some diffi-591 culties in the process. First, the user should make the registration and obtain 592

the corresponding ESGF account identified by the user's "OpenID" (https: 593 //en.wikipedia.org/wiki/OpenID) and password. Second, the user should 594 enrol in the groups in which the user is interested (e.g. CMIP5, CORDEX, 595 etc.). Without this step, the user can explore the available data, but can not 596 download it. After data search, the user can add the selected datasets to its 597 Data Cart which can be directly downloaded, dataset by dataset, using her/his 598 OpenId. Alternatively, several shell scripts (e.g. wget-YYYYMMDDHHMMSS.sh) 590 can be generated to download the selected dataset using the terminal. To use 600 these scripts the user should have the ESGF-Credentials installed in its home 601 (see e.g. https://meteo.unican.es/trac/wiki/ESGFGetCredentials or 602 https://github.com/ESGF/esgf-getcert for more details). However, note 603 that on the one hand, the credentials will be valid for just 72 hours and, on the 604 other hand, the scripts can not be modified or adapted to download other datasets. 605 To execute the script, the user can use a BASH shell code similar to the next: 606

```
DIR=~/.esg
USR=https://esgf-node/esgf-idp/openid/userName
PASS=userPassword
# Retrieve the credentials
export PATH=/root/java/oracle/jdk1.7.0_79/bin:$PATH
java -jar ./getESGFCredentials-0.1.4.jar --openid
        $USR --password $PASS --writeall --output $DIR
unset X509_USER_PROXY
# Executing the script in the terminal:
bash wget-YYYYMMDDhhmmss.sh
# Executing the script in a PBS queue
qsub -d $PWD -V wget-YYYYMMDDhhmmss.sh
```

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