

UNIVERSITÉ DE LAUSANNE

DOCTORAL THESIS

Software and Numerical Tools for Paleoclimate Analysis

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*A thesis submitted in fulfillment of the requirements
for the degree of Doctor of Science*

in the

The Davis Group
Institute of Earth Surface Dynamics (IDYST)

September 3, 2019

Declaration of Authorship

I, Philipp S. SOMMER, declare that this thesis titled, "Software and Numerical Tools for Paleoclimate Analysis" and the work presented in it are my own. I confirm that:

- This work was done wholly or mainly while in candidature for a research degree at this University.
- Where any part of this thesis has previously been submitted for a degree or any other qualification at this University or any other institution, this has been clearly stated.
- Where I have consulted the published work of others, this is always clearly attributed.
- Where I have quoted from the work of others, the source is always given. With the exception of such quotations, this thesis is entirely my own work.
- I have acknowledged all main sources of help.
- Where the thesis is based on work done by myself jointly with others, I have made clear exactly what was done by others and what I have contributed myself.

Signed:

Date:

“The purpose of computing is insight, not numbers.”

Richard Wesley Hamming

UNIVERSITÉ DE LAUSANNE

Abstract

Faculty of Geosciences and Environment (FGSE)
Institute of Earth Surface Dynamics (IDYST)

Doctor of Science

Software and Numerical Tools for Paleoclimate Analysis

by Philipp S. SOMMER

The Thesis Abstract is written here (and usually kept to just this page). The page is kept centered vertically so can expand into the blank space above the title too...

Acknowledgements

The acknowledgments and the people to thank go here, don't forget to include your project advisor...

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For/Dedicated to/To my...

Chapter 1

Introduction

1.1 Motivation

Climate science and in particular the study of past climates face an increasing need for the analysis, standardization and sharing of data. Scientists made huge efforts to explore climate archives throughout the world to investigate the evolution of the Earth's climate. In parallel, computational climate models grew in complexity and data output due to an increase of computational power and the availability of supercomputers. This generates new challenges for big data analysis that can only be solved by high quality and flexible software packages.

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The Neotoma Database, a global international database for paleoenvironmental proxies (Williams et al., 2018) currently lists XXX datasets with in total XXX samples for past 12'000 years, the Holocene. Such data collections enable large-scale reconstructions of past climates that however face considerable challenges. They mainly arise from the heterogeneity of the data and the necessity of further quality control and standardization. One key problem is the accessibility of data. A lot of data is not available in standardized relational databases and either held private, or is stored in less standardized archives such as PANGAEA, or is not available in a digital format at all. The latter often results in the need of digitizing the associated data from a published diagram, a tedious and imprecise task (Sommer et al., 2019). Additionally handling such a big heterogeneous data resource and analyzing its contents is a key challenge and requires flexible visualization resources that efficiently allow the querying of spatial data with heterogeneous time and meta data information.

3: Add reference.
<https://pangaea.de/>

4: Add reference.
EMPD paper

An additional challenge arises from the combination with numerical models that usually operate on a structured (Edwards, 2010; Treut et al., 2007) or unstructured grid with a fixed timestep. The development and analysis of such models requires visualization techniques that are interoperable with the specific data structure of the model (e.g. S. A. Brown et al., 1993; Rew and G. Davis, 1990) while still being flexible enough for general purposes and computations (Hoyer and Hamman, 2017; Sommer, 2017). Additionally it requires techniques to process observational data to make it comparable with climate models (Mauri et al., 2015) or to feed a model with the data using data assimilation of statistical models (Sommer and Kaplan, 2017).

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ICON

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per

In the following section 1.2 I will lay down the interest in the study of paleoclimates, both from the observational and the modellers perspective. This is continued by a section 1.3 which highlights the specific requirements and the historical development of software in paleo-science and concludes with section 1.3.3 that provides an overview on the contents of this thesis.

1.2 Learning from the Past – Why we study paleo-climates

Mankind is facing large infrastructural challenges during this century, such as the loss of biodiversity, an exponentially growing world population and an acceleration of growth and globalization of markets. They all interact with a global climate change that may lead to a new environment none of us ever experienced. Any future global planning has to account highly diverse responses that range from regional to continental scales. The complex (climate) system will enter a state that is significantly different from everything we had since the beginning of the satellite era in the 19th century, the beginning of global meteorological data acquisition.

Our knowledge about this new climate is therefore mainly based on computational Earth System Models (ESMs). They face the challenge of simulating a new climate based on our present knowledge of the interactions between the different compartments Ocean, Land and Atmosphere. Running such a model for the entire Earth with a reasonable resolution is therefore very cost-intensive and requires large computational resources. The validation of it becomes technically difficult considering the large amount of data output, and additionally conceptually difficult because of the aforementioned transition into a warmer world during the next century. We are entering a new state and it is questionable how well our models perform (Hargreaves et al., 2013; Karpechko, 2010; Ulden and Oldenborgh, 2006).

To evaluate their skill, we can only use our knowledge of the past climate from before the systematic measurement of temperature, precipitation, etc. These climates, also referred to as paleo-climates, provide the only opportunity to evaluate an ESM under conditions very different than today. paleo-climatic research has therefore been an integral part for climate sciences since the 80s (COHMAP Members, 1988; Joussaume and Taylor, 1995), particularly in the Paleoclimate Modelling Intercomparison Project (PMIP) (Braconnot et al., 2012, 2007a,b; Jungclaus et al., 2017; Kageyama et al., 2016; B. L. Otto-Bliesner et al., 2017).

The current geological period is the Quaternary. It is characterized by glacial-interglacial cycles mainly driven by orbital changes (Hays et al., 1976; Imbrie et al., 1993) that cause a varying insolation on the planet.

The end of this period can be used for data-model comparisons due to the availability of paleo-climate archives. It started with the Last Interglacial (LIG) about 127'000 years ago and was followed by the Last Glacial Maximum (LGM) at 21'000 years ago. The warming of the atmosphere in the following interglacial has been interrupted by a rapid cooling, called the Younger Dryas, between 12'900 and 11'700 years ago, which then let to the onset of the current epoch, the Holocene (Walker et al., 2009).

Add some background on the Holocene. How did it change (global mean temperature estimate?), how was the insolation? CO₂ effects, impact of the ice sheets during the early holocene, changes in altitude, large-scale atmospheric circulation, human influences.

This epoch is of particular interest because the continental setup is comparable to nowadays while still having a climate that is significantly different from present day. Additionally we have a large set of proxies available to quantify the climate, independent from the model estimates, and for the entire globe (Wanner et al., 2008)

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PMIP paper

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1.2.1 Proxy Data from the Holocene

Before 1850, there is almost no instrumental measurement of temperature. Instead we rely on archives such as lake sediments, glaciers, peat bogs, or speleothems that preserve climate proxies. The latter is a set of variables that are influenced by climate conditions and therefore allow an indirect measurement of climate parameters at ancient times, e.g. temperature, precipitation or sea-level. The most prominent proxies are isotopic compositions of $\delta^{18}\text{O}$ in glacial ice cores, marine sediments, peat bogs or speleothems; bio-ecologic assemblages such as pollen, chironomids or diatoms in lake sediments; foraminifera and alkenone in marine sediments; and the widths of tree rings.

The most abundant climate proxy, that I will also focus on in the next chapters, are pollen assemblages. It is the geographically most wide spread paleo-climate proxy (H. J. B. Birks and H. H. Birks, 1980) and has a long history in quantitative paleo-climatologic reconstructions (e.g. Bradley, 1985; Nichols, 1967, 1969).

The ability to serve as a proxy for the past arises from the chemically stable polymer sporopollenin, that allows it to be preserved over very long periods of time, in various environments such as lakes, wetlands or ocean sediments (Faegri et al., 1989; Havinga, 1967). Pollen are produced by seed-bearing plants (spermatophytes, Wodehouse, 1935) and as such have a high spatial continuity and prevalence. Their compositions (closely related to the surrounding vegetation) is highly dependent on the climate and allows the reconstruction of the latter through an inverse modelling approach.

The usefulness for large-scale data-model intercomparisons additionally arises from the existence of regional databases for fossil pollen assemblages. The earliest examples are the European Pollen Database (EPD) and North American Pollen Database (NAPD) that both started around 1990 and developed a similar structure in order to be compatible (Fyfe et al., 2009; Grimm, 2008). This led to the development of other regional pollen databases, such as the Latin American Pollen Database (LAPD) (LAPD, Flantua et al., 2015; Marchant et al., 2002) in 1994 or the African Pollen Database (APD Vincens et al., 2007) in 1996, and others (see Grimm, 2008). These attempts finally led to the development of the Neotoma database (Williams et al., 2018), a global multiproxy database that incorporates many of the regional pollen databases.

The use of the above-mentioned proxies, particularly pollen, for paleo-climate reconstruction has a long academic tradition in geology (Bradley, 1985) and provides the source of large-scale paleo-climatic reconstructions in number of different studies (B. A. S. Davis et al., 2003; Marsicek et al., 2018; Mauri et al., 2015; Neukom et al., 2019a,b). They however have multiple uncertainties, that are often difficult to estimate and to consider. The main challenge for a data-model comparison are dating uncertainties, but often also about the influence of seasonality on the proxy (e.g. whether it represents summer, winter or annual temperature) and the quality of the record. Another challenge is the proper handling of uncertainties of the inverse modelling approach, spatial coverage of the proxy (see chapter 3), and, considering pollen assemblages, the various naming schemes for pollen taxa that need to be considered for large-scale reconstructions.

1.2.2 Model Simulations of the Holocene

As mentioned in the earlier section 1.2, paleoclimate simulations of ESMs played an important role in previous intercomparisons. The Holocene analysis within past Paleoclimate Modelling Intercomparison Project (PMIP) versions focused mainly

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that North-US/South-
US discrepancy...

on the mid-Holocene around 6000 years before present, a time period with a different latitudinal and seasonal distribution of incoming solar radiation (insolation) but greenhouse gas concentrations similar to the preindustrial period (B. L. Otto-Bliesner et al., 2017). The main findings from previous intercomparisons are an underestimation of polar amplification in PMIP2 and PMIP3 models due to sea ice and vegetational feedbacks, and an underestimation of the north-south temperature gradient over Europe (Brewer et al., 2007; Basil A. S. Davis and Brewer, 2009; Intergovernmental Panel on Climate Change, 2014; Masson-Delmotte et al., 2006; Zhang et al., 2010).

The focus on only a short time slice (mainly due to the high computational costs for running an ESM over a large simulation period) however has several complications. Climate changes, i.e. the shift into a different climatic state, cannot be simulated and high dating uncertainties hinder a credible comparison of models and proxies. Therefore multiple recent studies published and proposed increasing efforts for transient model simulations, i.e. simulations that cover multiple millenia during the last deglaciation (Ivanovic et al., 2016) and the Holocene (B. L. Otto-Bliesner et al., 2017). Several studies used Earth System Models of Intermediate Complexity (EMICs) for transient simulations that cover parts of the last 12'000 years (e.g. Greigoire et al., 2015; Men viel et al., 2011; Roche et al., 2011) and a few used a global coupled ESM (Bette L. Otto-Bliesner et al., 2014; Varma et al., 2012, chapter 6). As stated by Weitzel et al., 2019, those model results can clarify the role of internal climate variability for Holocene temperature trends and large-scale patterns.

Despite the computational costs for running these models, technical challenges arise from the size of the data that easily exceeds the size of multiple Gigabyte per climatic variable with a monthly resolution. It requires software that is able to deal with data too large to fit into memory (see section 1.3.2 and chapter 2) and automated techniques to identify patterns in the data (see chapter 6).

1.3 Software for Paleoclimatology

The usage of software is crucial for the quantitative reconstruction of Earth's Climate. Paleoclimate research is facing an information overload problem and requires innovative methodologies in the realm of visual analytics, the interplay between automated analysis techniques and interactive visualization (Keim et al., 2008; Nocke, 2014). As such, a visual representation of the paleoclimate reconstruction has been essential for both, proxies (Bradley, 1985; Grimm, 1988; Nichols, 1967) and models (Böttinger and Röber, 2019; Nocke, 2014; Nocke et al., 2008; Phillips, 1956; Rautenhaus et al., 2018), although the visualization methods significantly differ due to the differences in data size and data heterogeneity.

The second important aspect for software and paleoclimate is the distribution of data to make it accessible to other researchers, the community and policy makers, which is commonly established through online accessible data archives and recently also through map-based web interfaces (Bolliet et al., 2016; Williams et al., 2018).

The following sections provide an overview on the different techniques used by modelers and palynologists to visualize and distribute their data and concludes with an introduction into Open-Source Software Development, which forms the basis of the software solutions that are presented later in this thesis (chapters 2, 3, and 4, and appendix C).

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32: Add reference.
cite some open-data publications

1.3.1 Sofware for Proxy Data Analysis, Visualization and Distribution

Due to the nature of stratigraphic data, proxies, especially pollen assemblages, are often treated as a collection of multiple time-series (one-dimensional arrays). The size of one dataset is generally small (in the range of kB) and can be treated as plain text files. Traditionally, numerical and statistical analysis are separated from the visualization.

In palynology, standard analytical tools are Microsoft Excel¹ and the R software for statistical computing (R Core Team, 2019). The latter also involves multiple packages for paleoclimatic reconstruction, such as `rioja` (Juggins, 2017) and `analogue` (Simpson, 2007; Simpson and Oksanen, 2019) or bayesian methods (Nolan et al., 2019; Tipton, 2017). Alternatively, desktop applications exist, such as `Polygon`² by Nakagawa et al., 2002 or the CREST software by M. Chevalier et al., 2014; Manuel Chevalier, 2019.

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It is a long-standing tradition to visualize stratigraphic data, and especially pollen data, in form of a stratigraphic (pollen) diagram (Bradley, 1985; Grimm, 1988). Especially during the 19th century, when it was not yet common to distribute data alongside a peer-reviewed publication, pollen diagrams were the only possibility to publish the entire dataset (see also chapter 3). The generation of these diagrams is usually based on desktop applications such as `C2` (Juggins, 2007), `Tilia`³ (Grimm, 1988, 1991). A more recent implementation into the `psyplot` framework (Sommer, 2017, chapter 2) is also provided with the `psy-strat` plugin⁴ (Sommer, 2019).

Raw pollen data is at present made available through web archives, such as PANGAEA⁵ or the National Climatic Data Center (NCDC) by the National Oceanic and Atmospheric Administration (NOAA)⁶ where researchers can create a DOI for their raw data. Collections of data, such as regional pollen databases or project specific collections (e.g. B. A. S. Davis et al., 2013; Whitmore et al., 2005) are usually published in one of the above-mentioned archives or associated with a publication. A different approach has been developed by Bolliet et al., 2016 to develop a small web application as an interface into the data collection, the *ClimateProxiesFinder* (Brockmann, 2016, chapter 4).

Outstanding compared to the previous data interfaces is the new infrastructure for the Neotoma database (Williams et al., 2018). It consists of the map-based web interface, the *Neotoma Explorer*⁷, a RESTful api⁸ that allows an interaction with other web services, the `neotoma` R package (Goring et al., 2015) and an interface into the `Tilia` software for stratigraphic and map-based visualizations (Williams et al., 2018). This rich functionality is, however, bound to the structure of Neotoma and as such, different from the Javascript-based approach developed in chapter 4 cannot easily be transferred to other projects.

1.3.2 The Development of Computational Climate Model Analysis

Software and computational numerics play a crucial role for our understanding of climate since the first General Circulation Models (GCMs) by Phillips, 1956 after

¹<https://products.office.com/en/excel>

²<http://polsystems.rits-paleo.com>

³<https://www.tiliaait.com/>

⁴<https://psy-strat.readthedocs.io>

⁵<https://pangaea.de/>

⁶<https://www.ncdc.noaa.gov/data-access/paleoclimatology-data>

⁷<https://apps.neotomadb.org/Explorer>

⁸<https://api.neotomadb.org>

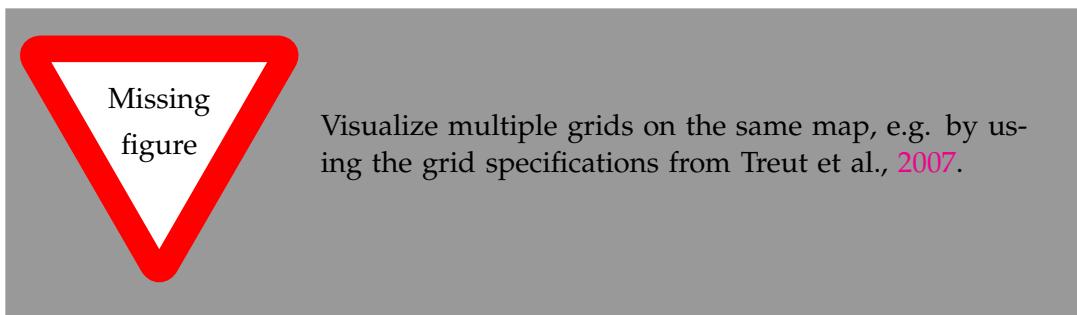


FIGURE 1.1: A selection of grid sizes and formats since the first IPCC report

world war II (Edwards, 2010; Lewis, 1998). The first simulations and analysis of GCMs where limited by the available computational facilities, the model by Phillips, 1956 for example operated on a 17×16 grid simulating a surface with the size of roughly one tenth of the Earth. The possibilities of climate modeling increased rapidly, mainly due to a drastic increase in computational capacity and the availability of supercomputers. This let to an increase in speed by a factor of roughly one million between 1970 and 2007, permitting an increase in model complexity, length of the simulations, and spatial resolution (Treut et al., 2007). In the past decade, unstructured grids raised more and more attention (Skamarock et al., 2012; Zängl et al., 2014) especially with the focus on *seamless prediction* (Bauer et al., 2015; Hoskins, 2012) that allows a refined grid resolution in selected regions of the earth (Rautenhaus et al., 2018).

The varying grids, multi-dimensionality and volume of the data requires visual analytic methodologies much different from what is used with proxy data (section 1.3.1) and much more diverse. In general, scientists tend to disentangle the numeric post-processing of climate model output (such as computing aggregated statistics in time or space dimension) and then visualize these aggregated results (Böttinger and Röber, 2019; Schulz et al., 2013). Common post-processing software are, for example Climate Data Operators (CDOs) (Schulzweida, 2019), netCDF Operators (NCOs) (Zender, 2008, 2016; Zender and Mangalam, 2007) and R (R Core Team, 2019), or more recently also python packages such as xarray (Hoyer and Hamman, 2017). The choice of method thereby depends on the scientists preference but also on the size of the data. Especially the analysis of transient model runs (section 1.2.2) requires software that is able to deal with data that is too big to fit into memory and requires parallel computation. Such an analysis can be done pursued with CDOs and xarray through it's interface with the parallel computing package dask (Dask Development Team, 2016; Rocklin, 2015) (see also chapter 6).

Rautenhaus et al., 2018 provide a detailed overview about how such a high amount of data is visualized. Methods range from 2D projection on a map to 3D interactive visualizations, depending on the background and knowledge of the researcher (Nocke, 2014). Nocke et al., 2008 recognize preference for script-based solutions such as Python, R or domain-specific languages such as NCL (D. Brown et al., 2012) that is still persistent today (Rautenhaus et al., 2018). Nocke, 2014, Schulz et al., 2013 and Rautenhaus et al., 2018 attribute this to the importance of comparability and reproducibility for research, and the usability in peer-reviewed publications. Therefore, 3D visualization, e.g. with ParaView (Ayachit, 2015), VAPOR (Clyne et al., 2007) or Avizo, are mainly used by visualization experts rather than

scientists (Nocke et al., 2008). However, Nocke, 2014 note that young researchers are more open for 3D visualization and especially with the newly emerging unstructured grids, they become more prominent. Besides psyplot (Sommer, 2017, chapter 2) and UV-CDAT, there exists to my knowledge no scripted method that easily visualizes climate model data on unstructured grids, without the need for interpolation to a rectilinear grid. These have however been implemented for ParaView (Röber et al., 2015) and Vapor (Jubair et al., 2015) and new interfaces into VTK have also been developed by Sullivan and Trainor-Guitton, 2019.

[Look into ibid](#)

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1.3.3 Methods and Workflows in Open-Source Software Development

The importance and necessity of software for visualization and data analysis led to the development of the software packages presented in this thesis. Most of them are written in the programming language Python (Perez et al., 2011), on the one hand due to my personal preference, but mainly due to the recent developments in out-of-core computing with the establishment of xarray and dask (Dask Development Team, 2016; Hoyer and Hamman, 2017; Rocklin, 2015). Another important reason, especially for psyplot (chapter 2) and straditize (chapter 3) was the availability of a highly flexible and stable package for graphical user interfaces, PyQt, and the comparably simple possibility to implement an in-process python console into the PyQ5 application that allows to handle the software functionalities both, from the command line and from the GUI.

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Modern Free and Open-Source Software (FOSS) development is not only about making the source code available, but rather about providing a sustainable and maintainable package that allow continuous and transparent development under the aspect of rapidly evolving environment. In the following sections, I will introduce the most important FOSS development concepts (e.g. Shaw, 2018; Stodden and Miguez, 2014) and the necessary vocabulary. These concepts are used by many of the well-established software packages, such as matplotlib (Hunter, 2007), numpy (T. E. Oliphant, 2006), and scipy (Jones et al., 2001).

Version Control

Version control systems record changes to a file and enables the user to roll-back to previous versions of it. The usage of a such a system is inevitable for sustainable FOSS packages. It enables contributions by other FOSS developers and the usage through external packages.

The packages I present in the following chapters are hosted on Github⁹, a freely available web platform for hosting projects that are managed with git (Chacon et al., 2019).

Version control with git has a specific terminology. Central aspects are *repositories* (project folders), *commits* (change of the project files), *issues* (bug reports), *branches* and *forks* (copies of the (main) project), and *pull requests* (contributions to a project). The following list explains this vocabulary in a bit more detail, a more complete list is provided by in Github, Inc., 2019.

Repositories are the most basic elements of git and Github. It can be compared to a folder that contains all the necessary files associated with a project (e.g. the source code and documentation of a software package). It also contains all the different versions (revisions) of the project files.

⁹The packages are available at <https://github.com/Chilipp>. Other potential platforms for version control are sourceforge (<https://sourceforge.net>) and Bitbucket (<https://bitbucket.org>)

Commits or revisions track the changes in the repository. Each commit is a change to a specific file (or a set of files) that is associated with a unique ID and a message of the author about to describe the changes.

Issues are suggested improvements, bug reports or any other question to the repository. Every issue has a associated discussion page the topic can be discussed between repository owners and the users.

Branches are parallel versions of a repository. Often one incorporates new developments into a separate branch that does not affect the main version of the repository (the *master* branch) and merge the two versions when the new developments are fully implemented.

Forks are copies of repositories. When someone wants to contribute to a software package (repository) that does not belong to him, he can *fork* (copy) it, implement it's changes, and then create a *pull request* to contribute to the official version. Different from a branch, that is a (modified) copy of another branch, forks are copies of the entire repository, i.e. all existing branches.

Pull request are the proposed changes to a repository. One can create a fork of the repository from someone else, implement changes in this fork and then create a pull request to merge it into the original repository. Every pull request has an associated discussion page that allows the repository owner to moderate and discuss the suggested changes.

Webhooks are general methods for web development. Github can trigger a hook to inform a different web service (such as a Continuous Integration (CI) (section 1.3.3)) that a repository has changed or that someone contributed in a discussion. In chapter 4 we use Github webhooks for a automated administration of a repository.

Automated Tests, Test Coverage and Continuous Integration

The most important aspect for FOSS development, especially considering the rapid evolution of this area, is the existence of automated tests. One distinguishes unit tests (test of one single routine) and integration tests (tests of one or more routines within the framework) (Shaw, 2018). The boundary between the two tests is rather vague and what is more appropriate highly depends on the structure of the software that is supposed to be tested. For complex frameworks (such as psyplot or straditz), integration tests are needed to ensure the operability within the framework. Other more simple software packages, (such as docrep or model-organization, see appendix C.2) go well with unit tests only.

Another good standard for such an test suite is to use an automated test discovery tool (e.g. the Python unittest package (Python Software Foundation, 2019) or pytest (Krekel et al., 2004)) that also reports the test coverage (i.e. the fraction of the code that is tested by the test suite). These functionalities are then implemented on a CI service, such as Travis CI¹⁰, Appveyor¹¹ or CircleCi¹² that are integrated into the Github repository (section 1.3.3). Every commit to the Github repository or a new pull requests then triggers the tests. This transparently allows to ensure the

¹⁰<https://travis-ci.org/>

¹¹<https://appveyor.com>

¹²<https://circleci.com/>

operability of the software, and the test coverage report ensures that the newly implemented functionality is properly tested. A software development concept that is build entirely on that is the test-driven development. Within this framework, new features are implemented by starting with the test that should be fulfilled by the new feature and then improving the software until this test pass (Beck, 2002).

Automated Documentation

Documentation is the key aspect of a sustainable software and much of the geo-scientific code has a lack of proper documentation (based on personal experience). For the software in this thesis, for different levels of the documentation play an important role:

The Application programming interface (API) documentation is meant to document the major parts of the software code that is subject to be used by external scripts or packages. It is usually implemented in the code and documents the essential subroutines and methods of the software.

The Graphical User Interface (GUI) documentation provides help for the most high-level functionality for the software. The GUI is a user interface into the software through graphical elements (such as buttons, checkboxes, etc.). Unlike the API documentation, it should not require knowledge about programming.

The contributing and/or developers guide is targeting other software developers that might want to contribute to the software package. This document states how other software developers should contribute to the software and introduces the central structural aspects and frameworks of the software.

The manual (or also commonly referred to as *the* documentation) is the document that contains all necessary information for the software, such as installation instructions, tutorials, examples, etc.. It often includes some (or multiple) of the above parts.

The documentations for the software in this thesis have been automatically generated with Sphinx, a Python tool to generate documentations in various different formats (such as HTML, PDF, etc.) (Hasecke, 2019; Perez et al., 2011). It is also implemented as a webhook into the Github repository (see section 1.3.3) to automatically generate an up-to-date documentation of the software for each commit to the Github repository. This provides an additional automated test for the software, and especially its high-level-interface, in addition to the automated test suite described above (section 1.3.3). Most of the manuals are hosted and build online with the free services offered by [readthedocs.org](#).

Distribution through package managers and virtual environments

FOSS software is meant to be extensible and to build upon other FOSS packages. This requires an accurate and transparent handling of its dependencies and requirements which is usually provided through the so-called packaging of the software (e.g. Torborg, 2016). There exists a variety of package managers and the choice most often depends on the framework of the software.

The software in this thesis is mainly distributed via two systems. The first one is python's own package manager *pip* which is based on the packages uploaded to [pypi.org](#). The second one which got increasing importance during the recent past is

the open-source Anaconda Distribution¹³. Both work on multiple operating systems (Windows, Linux and Mac OS), but the Anaconda Distribution contains also non-python packages (e.g. written in C or C++) for which the Python packages rely on, and it contains a rich suite of r-packages.

One step further, compared to package managers, are the distribution of virtual environments. These systems do not only provide the software, but also a full operating system and the installed dependencies. A popular platform (used also for the Eurasian Modern Pollen Database (EMPD) database) is provided through so-called Docker containers¹⁴. Compared to package managers, this system has the advantage of simplifying the installation procedure for the user because he only has to download the corresponding docker image. The docker image itself then runs independent of the local file system in a separate isolated mode.

1.4 Challenges tackled in this thesis

I present several new tools in this thesis that tackle the aspects described in the previous sections. It is divided into two parts: Part I are the software chapters 2, 3 and 4 that introduce new packages developed for paleoclimate analysis. Part II consists of the analysis chapters 5 and 6 that address two use-cases tackling the combination of observations and models for an informed paleoclimate understanding.

The first part starts with the visualization framework psyplot in chapter 2, a suite of python packages that are designed for interactive visual analysis of data both from a GUI and the command line. The scope of this software is not limited to paleoclimate analysis and serves a more general purpose. As such, it serves as a base infrastructure for many of the topics described in the other chapters.

Straditize, described in the next chapter 3, addresses the problem of gathering paleo-climate information that has been collected during the pre-digital area. This software is a semi-automated digitization package for stratigraphic diagrams, particularly pollen diagrams. Straditize is built on top of psyplot and its GUI and as such provides a rich interactive documentation and visualization methods of the software tools.

Chapter 4 covers the last aspect of software usage for paleoclimate data: data distribution. In this chapter I describe new infrastructural tools for the sustainable management of a community-driven pollen database, the Eurasian Modern Pollen Database (EMPD). They consist of a flexible and lightweight map-based web interface, the EMPD-viewer, into the data and a webserver for an automated administration of the database. Within this section, I also present another use case for the EMPD-viewer that is adapted to a large northern-hemispheric database of fossil and modern pollen records.

The second part starts with the weather generator GWGEN in chapter 5, a statistical model that uses modern relationships in observational data to inform large-scale paleo climate models with temporally downscaled temperature, precipitation, cloud cover and wind speed records.

Finally, in chapter 6 I investigate the question to what extent large-scale atmospheric circulation features can be estimated from proxy data. In this analysis I analyze the long-term stability of spatial correlation patterns between surface temperature and northern hemispheric teleconnections based on three ESMs.

¹³<https://www.anaconda.com>

¹⁴<https://www.docker.com>

This thesis finishes with the conclusions in chapter 7 which summarizes the new tools and findings and provides an outlook for the further development of the methods presented. In the Appendix I present another work that has developed in a co-operation which is also based on the infrastructural tools from psyplot and GWGEN (appendix A), and I provide a list of the publications during my thesis (appendix B) and an overview about all the software packages that have been developed (appendix C).

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Part I New Software Tools for Paleoclimate Analysis

Chapter 2

Psyplot

A flexible framework for interactive data analysis

Need to write chapter 2

- Summary (from JOSS Paper)
- Other visualization frameworks (short review)
- The psyplot framework design
- Integration into a graphical user interface

Chapter 3

Straditize

A digitization software for pollen diagrams

Need to write chapter 3

- quaternary paper
- straditize builds upon the psyplot GUI
- fill the gaps for large-scale climate reconstructions

Chapter 4

The EMPD- and POLNET web-interface to pollen data

Need to write chapter 4

- quaternary paper
- straditize builds upon the psyplot GUI
- fill the gaps for large-scale climate reconstructions

Part II Numerical Analysis of Paleoclimate Data

Chapter 5

GWGEN v1.0

A globally calibrated scheme for generating daily meteorology from monthly statistics

Abstract. While a wide range of earth system processes occur at daily and even sub-daily timescales, many global vegetation and other terrestrial dynamics models historically used monthly meteorological forcing, both to reduce computational demand and because global datasets were lacking. Recently, dynamic land surface modeling has moved towards resolving daily and subdaily processes, and global datasets containing daily and sub-daily meteorology have become available. These meteorological datasets, however, cover only the instrumental era of the last ca. 120 years at best, are subject to considerable uncertainty, and represent extremely large data files with associated computational costs of data input/output and file transfer. For periods before the recent past or into the future, global meteorological forcing can be provided by climate model output, but the quality of these data at high temporal resolution is low, particularly for daily precipitation frequency and amount. Here we present GWGEN, a globally applicable statistical weather generator for the temporal downscaling of monthly climatology to daily meteorology. Our weather generator is parameterized using a global meteorological database and simulates daily values of five common variables: minimum and maximum temperature, precipitation, cloud cover, and wind speed. GWGEN is lightweight, modular, and requires a minimal set of monthly mean variables as input. The weather generator may be used in a range of applications, for example, in global vegetation, crop, soil erosion, or hydrological models. While GWGEN does not currently perform spatially autocorrelated multi-point downscaling of daily weather, this additional functionality could be implemented in future versions.

5.1 Introduction

The development of the first global vegetation models in the 1970's (e.g., Helmut Lieth, 1975) brought about the demand for meteorological forcing datasets with global extent and relatively high spatial resolution, e.g., $1^\circ \times 1^\circ$. While a global weather station-based monthly climate dataset was available at this time (Walter and H Lieth, 1967), limitations in computers and storage allowed only the simplest treatment of these data. The first global simulations of the net primary productivity of the terrestrial biosphere (Helmut Lieth, 1975), thus used rasterized polygons of annual meteorological variables that had been crudely interpolated from the station-based climatology. A decade later saw the development of better computers and more sophisticated global vegetation models (I. C. Prentice et al., 1992; I. Prentice, 1989)

that recognized the need for forcing at a sub-annual timestep and development of these models was done in parallel with the first global, gridded high resolution (0.5°) monthly climatology (Leemans and Cramer, 1991). At the time, monthly meteorological data was the only feasible global data that could be produced, in terms of the raw station data available to feed the interpolation process, the processing time required to produce gridded maps, and the data storage and transfer capabilities of contemporary computer systems and networks. Global gridded monthly climate data thus became the standard for not only large-extent vegetation modeling (A. Haxeltine and I. C. Prentice, 1996; Alex Haxeltine et al., 1996; J. O. Kaplan et al., 2003; Kucharik et al., 2000; Woodward et al., 1995), but also for a wide range of studies on biodiversity and species distribution (e.g., Elith et al., 2006), vegetation trace gas emissions (e.g., Guenther et al., 1995), and even the geographic distribution of human diseases (e.g., Bhatt et al., 2013).

Over subsequent years, the global gridded monthly climate datasets were improved (New et al., 1999, 2002), developed with very high spatial resolution (Hijmans et al., 2005), and expanded beyond climatological mean climate to cover continuous timeseries over decades (Harris et al., 2014; Mitchell and P. D. Jones, 2005; New et al., 2000). The latter was an essential requirement for forcing dynamic global vegetation models (DGVMs) (e.g., Sitch et al., 2003). However, despite increasing quality, spatial resolution, and temporal extent in these datasets, the basic time step remained monthly, partly for legacy reasons — models had been developed in an earlier era subject to computational limitations and therefore used a monthly timestep for efficiency even if this was no longer strictly a constraint — and partly because of the challenge in developing a global, high-resolution climate dataset with a daily or shorter timestep still presented a major data management challenge.

On the other hand, there was increasing awareness that accurate simulation of many earth surface processes required representation of processes at a shorter-than-monthly timestep. Global simulation of surface hydrology (Gerten et al., 2004), crop growth (Bondeau et al., 2007), or biogeophysical processes (Krinner et al., 2005) needed sub-monthly forcing to produce reliable results. To address this need for better forcing data, two main approaches were taken: either monthly climate data were downscaled online using a stochastic weather generator (e.g., Pfeiffer et al., 2013), or a sub-daily, high-resolution, gridded climate timeseries was generated directly by merging high-temporal-resolution reanalysis data (e.g., NCEP, 6h, 2.5°) with high-spatial-resolution monthly climate data (e.g., CRU, 0.5°). The latter process resulted in the CRUNCEP dataset (Viovy and Ciais, 2016; Wei et al., 2014), which, while global, is large even by modern standards (ca. 350 Gb), is not available at spatial resolution greater than 0.5° , and covers only the period 1901-2014.

Forcing data for global vegetation and other models with shorter than monthly resolution at higher spatial resolutions than 0.5° , or for any other period than the last ca. 120 years, e.g., for the future or the more distant past, may therefore only be available through downscaling techniques. One approach to overcome the limitations of currently available datasets could be to use GCM output directly, however, most GCM output currently available does not have greater than 0.5° spatial resolution, with the current generation of GCMs typically approaching ca. $1^\circ \times 1^\circ$. Furthermore, there is a general observation that daily meteorology produced by GCMs is not realistic, particularly for precipitation (Dai, 2006; Stephens et al., 2010; Sun et al., 2006). An alternative approach is, therefore, to perform temporal downscaling on monthly meteorological data using a statistical weather generator.

Statistical weather generators were first developed primarily for crop and hydrological modeling at the field to catchment scale (Richardson, 1981; Woolhiser

and Pegram, 1979; Woolhiser and Roldan, 1982). The weather generator was parameterized using daily meteorological observations at one or more weather stations close to the area of interest, although some attempts were made to generalize the parameterization over larger, sub-continental regions (e.g., D. S. Wilks, 1998, 1999b; Woolhiser and Roldán, 1986). Locally parameterized weather generators have been applied to a very wide range of studies (D. S. Wilks and Wilby, 1999; Daniel S. Wilks, 2010), and enhanced to include additional meteorological variables beyond the original precipitation, temperature, and solar radiation (e.g., Parlange and Katz, 2000). Applications of a weather generator at continental to global scales was still limited, however, because of the need to perform local parameterization.

The need to simulate daily meteorology in regions of the world with short, unreliable, or unavailable daily meteorological timeseries brought about the realization that certain features of weather generator parameterization might be generalized across a range of climates (S. Geng et al., 1986; Shu Geng and Auburn, 1987). This ultimately led to the development of globally applicable weather generators (Friend, 1998), and their incorporation in DGVMs (Bondeau et al., 2007; Gerten et al., 2004; Pfeiffer et al., 2013). The original global parameterization (S. Geng et al., 1986) of these weather generators was, however, limited to seven weather stations, mostly in the temperate latitudes. Friend, 1998 does not publish the parameters used in his global weather generator, but we assume these were the same as the original Shu Geng and Auburn, 1987 and S. Geng et al., 1986 models. Given the availability of 1) large datasets of daily meteorology, and 2) computers powerful enough to process these data, we therefore decided that it would be valuable to revisit these parameterizations, perform a systematic and quantitative evaluation of the resulting down-scaled meteorology, and potentially improve our ability to perform monthly-to-daily downscaling of common meteorological variables with a single, globally applicable parameterization.

In the following sections we describe Global-WGEN (GWGEN), a weather generator parameterized using more than 50 million daily weather observations from all continents and latitudes. We demonstrate how updated schemes for simulating precipitation occurrence and amount, and for bias correcting wind speed, further improve the quality of the model simulations. We perform an extensive model evaluation and parameter uncertainty analysis in order to settle on a parameter set that provides the most accurate, globally applicable results. We comment on the limitations of the model and priorities for future research. GWGEN is an open-source, stand-alone model that may be incorporated into any number of models designed to work at global scale, including, e.g., vegetation, hydrology, climatology, and animal distribution models.

5.2 Model description

GWGEN requires the following six monthly summary values as input: 1) total monthly precipitation, 2) the number of days in the month with measurable precipitation (i.e., wet days), 3-4) monthly mean daily minimum and maximum temperature, 5) mean cloud fraction, and 6) wind speed. The model outputs are the same variables at daily resolution. This section summarizes the basic workflow in the model which is also shown schematically in Figure 5.1 and Algorithm 1.

The first approximation of the daily variables comes from smoothing the monthly time series using a mean-preserving algorithm (Rymes and Myers, 2001).

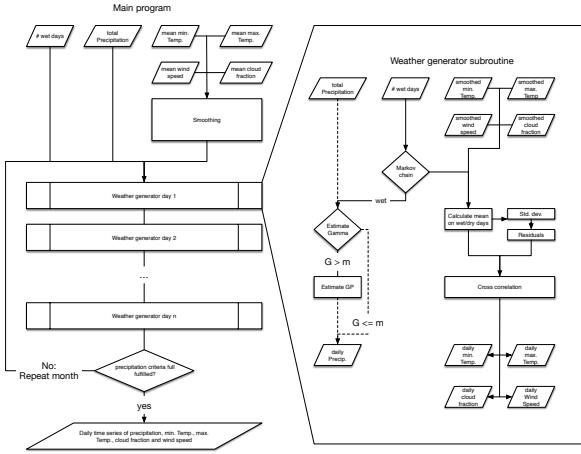


FIGURE 5.1: Schematic workflow of GWGEN. After smoothing the monthly input, the Markov Chain is used to decide, whether it is a dry or a wet day. If it is a wet day, we draw a random number from the Gamma-GP distribution. Furthermore, the other means of the variables ($\bar{T}_{\min/\max}, \bar{c}, \bar{w}$) are adjusted and their daily values are calculated using the estimated standard deviations and residuals. The wind speed furthermore undergoes a square root transformation before applying the cross correlation and in the end is corrected using the bias correction. A quality check in the end restricts our model to be within a 5% range of the observed total precipitation and to replicate the number of wet days from the input.

For precipitation we then first use the Markov Chain approach (section 5.3.2) to decide the wet/dry state of the day. If it is a wet day, we calculate the gamma parameters using the equations (5.7) and (5.8). The resulting distribution allows us to draw a random number, the precipitation amount of the currently simulated day. If we are above the threshold μ , we draw a second random number from the GP distribution parameterized via equation (5.9) and the chosen GP shape.

The next step modifies the means of temperature, wind speed and cloud fraction depending on the wet/dry state of the day (lines 11 and 15 in algorithm 1). After that, we use the cross-correlation approach described in Richardson, 1981 (lines 18 - 20 and Equation 5.3.2) and calculate the daily values of these variables. Finally we use the quantile-based bias correction described in section 5.3.4 to correct the simulated wind speed.

We restrict the weather generator to reproduce the exact number of wet days (± 1) as the input and to be within a 5% range of the total monthly precipitation (with a maximum allowed deviation of 0.5 mm). If the program cannot produce these results, the procedure described above is repeated (see line 4).

5.3 Model development

GWGEN is based on the WGEN weather generator (*ibid.*), using the method of defining the model parameters based on monthly summaries described by S. Geng et al., 1986 and Shu Geng and Auburn, 1987. GWGEN diverges from the original WGEN by using a hybrid-order Markov chain to simulate precipitation occurrence (D. S. Wilks, 1999a), and a hybrid Gamma-GP distribution (Furrer and Katz, 2008; Neykov et al., 2014) to estimate precipitation amount. Temperature, cloud cover,

Algorithm 1 Basic workflow of GWGEN

Require: monthly precipitation P_{in} [mm], cloud cover fraction c_{in} , minimum ($T_{\min,\text{in}}$ [$^{\circ}\text{C}$]) and maximum ($T_{\max,\text{in}}$ [$^{\circ}\text{C}$]) temperature, wind speed w_{in} [m/s], number of wet days n_{in}

Output: daily P_i [mm/d], c_i , T_i [$^{\circ}\text{C}$], w_i [m/s] and the wet/dry state $s_i \in \{0, 1\}$

- 1: **for** month m in *input* **do**
- 2: smooth the monthly data using Rymes and Myers, 2001
- 3: Set $j = 0$, $\chi = 0$
- 4: **while** $j \equiv 0$ or $|\sum_{d_i \in m} P_i - P_{\text{in}}| > \min(5\% \cdot P_{\text{in}}, 0.5\text{mm})$ or $|n_{\text{sim}} - n_{\text{in}}| > 1$ **do**
- 5: **for** day d_i in m **do**
- 6: Calculate p_{11}, p_{101}, p_{001} after equations (5.1) - (5.3) using n {Precipitation occurrence after D. S. Wilks, 1999a}
- 7: Use the Markov chain to determine whether d_i is wet ($s_i = 1$) or dry ($s_i = 0$)
- 8: **if** $s_i = 1$ **then**
- 9: Calculate θ, α and σ via eq. (5.7)-(5.9) {Precipitation amount after Neykov et al., 2014}
- 10: Draw a random number P_i from the Gamma-GP distribution, eq. (5.6)
- 11: Set $T_{\min,i} = T_{\min,\text{wet}}$, $T_{\max,i} = T_{\max,\text{wet}}$, $c_i = c_{\text{wet}}$, $w_i = w_{\text{wet}}$ from eq. (5.10) and (5.12) and tables 5.1, 5.3
- 12: Set $\sigma_{T_{\min,i}} = \sigma_{T_{\min,\text{wet}}}$, $\sigma_{T_{\max,i}} = \sigma_{T_{\max,\text{wet}}}$, $\sigma_{w,i} = \sigma_{w,\text{wet}}$, $\sigma_{c,i} = \sigma_{c,\text{wet}}$ from eq. (5.11), (5.13) and (5.14) and tables 5.1, 5.2, 5.3
- 13: **else**
- 14: Set $P_i = 0$ mm/d
- 15: Set $T_{\min,i} = T_{\min,\text{dry}}$, $T_{\max,i} = T_{\max,\text{dry}}$, $c_i = c_{\text{dry}}$, $w_i = w_{\text{dry}}$ from eq. (5.10) and (5.12) and tables 5.1, 5.3
- 16: Set $\sigma_{T_{\min,i}} = \sigma_{T_{\min,\text{dry}}}$, $\sigma_{T_{\max,i}} = \sigma_{T_{\max,\text{dry}}}$, $\sigma_{w,i} = \sigma_{w,\text{dry}}$, $\sigma_{c,i} = \sigma_{c,\text{dry}}$ from eq. (5.11), (5.13) and (5.14) and tables 5.1, 5.2, 5.3
- 17: **end if**
- 18: Draw 4 normally distributed random numbers $\epsilon \in \mathbb{R}^4$ {Cross correlation after Richardson, 1981}
- 19: Set the residuals $\chi_i = (\chi_{T_{\min}} \quad \chi_{T_{\max}} \quad \chi_c \quad \chi_w) = A\chi_{i-1} + B\epsilon \in \mathbb{R}^4$ with A and B from eq. (5.17)
- 20: Calculate daily variables via

$$T_{\min,i} = \chi_{T_{\min}} \cdot \sigma_{T_{\min,i}} + T_{\min,i} \quad c_i = \chi_c \cdot \sigma_{c,i} + c_i$$

$$T_{\max,i} = \chi_{T_{\max}} \cdot \sigma_{T_{\max,i}} + T_{\max,i} \quad w_i = (\chi_w \cdot \sqrt{\sigma_{w,i}} + \sqrt{w_i})^2$$
- 21: Apply bias correction w (eq. (5.23))
- 22: $j = j + 1$
- 23: **end for**
- 24: **end while**
- 25: **end for**

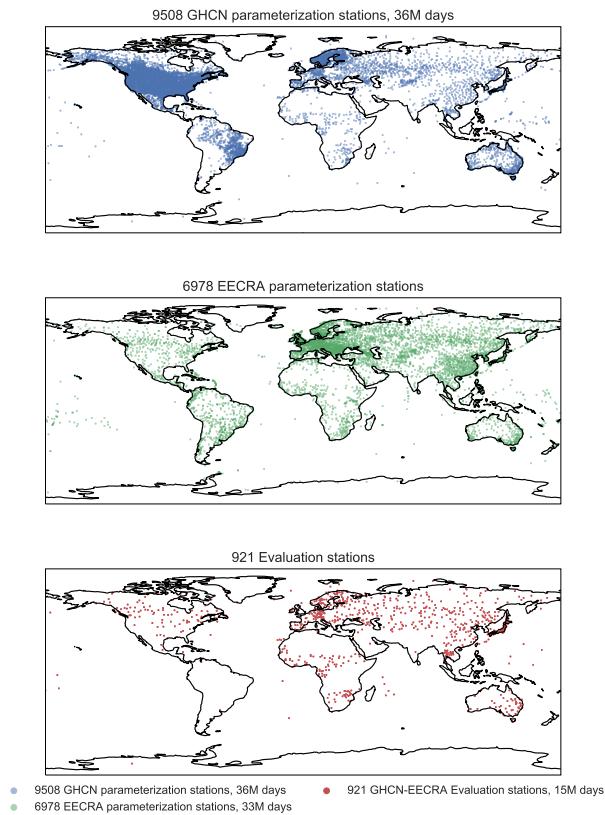


FIGURE 5.2: Weather stations used for parameterization and evaluation of the weather generator. The uppermost panel shows the locations of the stations used for parameterizing precipitation and temperature, the middle panel shows the stations for cloud fraction and wind speed, as well as for calculating the cross correlations between temperature, cloud fraction, and wind speed. The lower plot shows the location of the stations used to evaluate the model, which were excluded from the parameterization stations.

and wind speed are calculated following (Richardson, 1981), using cross correlation and depending on the wet/dry-state of the day. We further add a quantile-based bias correction for wind speed and minimum temperature, which improves the simulation results significantly.

In the following subsections, we first describe the global weather station database used to develop and evaluate the model, then describe the underlying relationships that we use to define GWGEN’s parameters.

5.3.1 Development of a global weather station database

To parameterize GWGEN, we assembled a global dataset of daily meteorological observations. Precipitation and minimum and maximum daily temperature come from the daily Global Historical Climatology Network (GHCN-Daily) database (Menne et al., 2012a,b). The GHCN-Daily consists of observations collected at ca. 100'000 weather stations on all continents and many oceanic islands. As the GHCN-Daily stations are highly concentrated in some parts of the world, particularly in the conterminous United States, we selected stations for our study using a geographic anti-aliasing filter to avoid an especially strong geographic bias in the generation of the

model parameters. Dividing the world up into a 0.5° grid, we selected the single station with the longest record in each cell, if one was present. While the GHCN-Daily units for precipitation have a nominal precision of 0.1 mm, several of the stations in the United States reported precipitation in fractions of an inch, which were later converted to mm. To ensure uniform precision across all of our calibration stations — this was particularly important when generating the probability density functions for precipitation amount — we selected only those GHCN-Daily stations where all precipitation amounts between 0.1 and 1.0 mm d $^{-1}$ were reported in the record. This resulted in 9508 stations covering all continents, although the distribution is strongly heterogenous, with the majority of the stations in North America, despite our geographic filter (Figure 5.2, top panel). For cloud cover, windspeed, and to calculate cross-correlations between temperature, cloud cover, and windspeed, we used the Extended Edited Cloud Report Archive (EECRA) database (Hahn and Warren, 1999). The geographic distribution of the 6978 EECRA stations we selected is different than the GHCN-Daily, with more stations in Europe (Figure 5.2, middle panel), but overall a relatively similar number of stations were used from both datasets. For the observations from both GHCN-Daily and EECRA, we made one additional filtering step, selecting only complete months, i.e., months with no days having missing observations, for further processing. In total, our database of daily meteorological observations used in the model parameterization contains ca. 69 million individual records.

Finally, we reserved some weather station records for model evaluation that were not used for model parameterization. These were individual stations, or two stations separated by a maximum distance of 1 km, where all of the daily meteorological variables that GWGEN simulates (P , T_{\min} , T_{\max} , c , w) were recorded on the same dates in the EECRA database. This merged selection from EECRA and GHCN resulted in a set of 921 stations representing ca. 15 million daily records, with observations on all continents, although the geographic distribution is once again highly heterogeneous, with a particularly high density of stations in Japan and Germany (Figure 5.2, bottom panel).

5.3.2 Parameterization

Precipitation occurrence

Following S. Geng et al., 1986, we expect to find a good relationship between the fraction of days in a month with measurable precipitation and the probability that any given day will be wet. Following D. S. Wilks, 1999a we use a hybrid-order model that retains first-order Markov dependence for wet spells but allows second-order dependence for dry sequences; this hybrid-order scheme has been shown to be a good compromise between performance and simplicity. To parameterize the precipitation occurrence part of the model, we thus calculated transition probabilities for a wet day being followed by a wet day (p_{11}), for a wet day being followed by a dry day being followed by a wet day (p_{101}) and for two dry days being followed by a wet day (p_{001}). We perform this analysis on a station and month-wise basis, i.e., we first extract each of the (complete) Januaries, Februaries, etc. for a given station, and then merge all of the Januaries (Februaries, Marches, etc...) for this station into a single series representing each month. Merging months over several years is particularly important for stations that have relatively little precipitation in a given month; for example, it could take several years of observations to observe a single

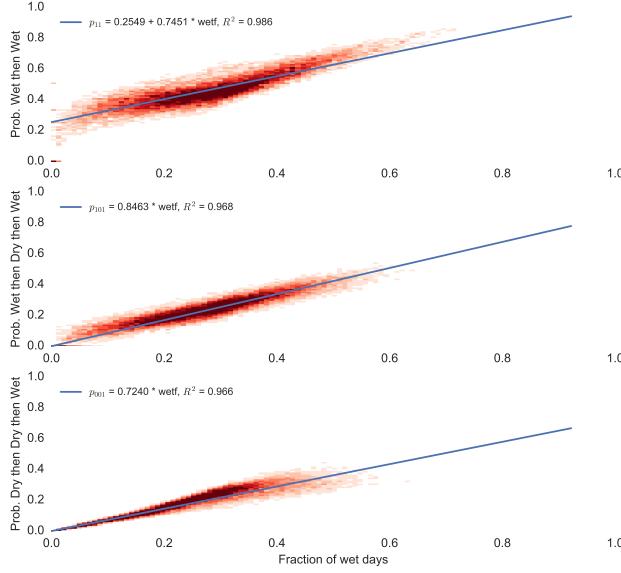


FIGURE 5.3: Transition probabilities vs. wet fraction. The red density plot in the background shows the density of the observations, and the blue lines are the linear regression line of the probability against the wet fraction. The fit for the p_{11} transition probability was forced to the point $(1, 1)$, the others were forced to $(0, 0)$. The underlying data for the fits correspond to the means of the the multi-year series for each station.

(p_{101}) event. The final transition probabilities were then regressed against the fraction of days in the month with precipitation, which show the characteristic linear relationship described by S. Geng et al., 1986 (Figure 5.3).

Because the transition probabilities (p_{001}) and (p_{101}) must be zero by definition when the fraction of wet days (f_{wet}) is zero, i.e., a completely dry month, we force the linear regression between these quantities to pass through the origin. Likewise, we require the regression line for (p_{11}) to equal 1 when f_{wet} is 1. One has to note, however, that this methodology artificially increases the R^2 coefficient for the fit because we fix the intercept (see for example Gordon, 1981).

The analysis results in the the following relationships:

$$p_{11} = 0.2549 + 0.7451 \cdot f_{\text{wet}} \quad (5.1)$$

$$p_{101} = 0.8463 \cdot f_{\text{wet}} \quad (5.2)$$

$$p_{001} = 0.7240 \cdot f_{\text{wet}}. \quad (5.3)$$

In the weather generator (see line 6 in algorithm 1) we determine if any given day will have precipitation by calculating the appropriate probability density function selected from equations (5.1)-(5.3) on the basis of the precipitation state of the previous day (or two). Comparing the calculated probability from the selected equation with a random number $u \in [0, 1]$, a precipitation day is simulated if u is greater than its corresponding probability.

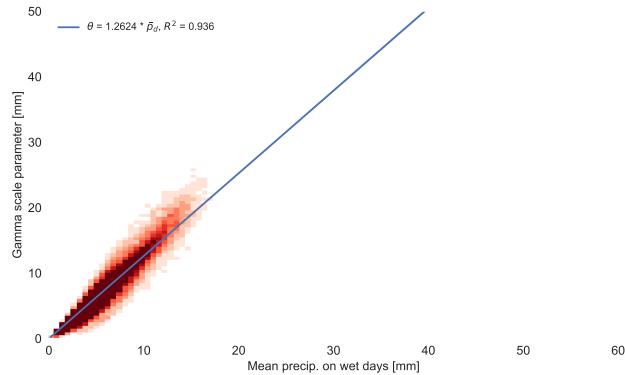


FIGURE 5.4: Mean precipitation - Gamma scale relationship. The blue line represents the best fit line of the mean precipitation on wet days to the estimated gamma scale parameter of the corresponding distribution. Each data point corresponds to one multi-year series of one month for one station.

Precipitation amount

Following the original WGEN (Richardson, 1981), GWGEN disaggregates precipitation amount using a statistical distribution. A number of different probability density functions have been used to estimate precipitation amount in weather generators including, e.g., single exponential or mixed exponential, one or two parameter gamma, or Weibull distribution (D. S. Wilks and Wilby, 1999). The strong relationship between the gamma scale parameter and the mean precipitation on wet days noted by S. Geng et al., 1986 makes generation of precipitation amounts with only monthly input data feasible. It is based upon the fact that the expected value of a gamma random variable equals the product of its two parameters. i.e $E(\Gamma) = \alpha\theta$. The gamma distribution, however, shows poor performance in simulating high-precipitation events consistent with observations. Furrer and Katz, 2008 and Neykov et al., 2014 suggest that a hybrid probability density function, based on both gamma and the generalized pareto (GP) distribution, has superior accuracy in simulating extreme precipitation events when compared to gamma alone. Because of its superior accuracy and ease of implementation, we therefore adopt the hybrid gamma-GP distribution for simulating precipitation amount in GWGEN.

The probability density function (pdf) of the gamma distribution is defined as

$$f(x) = \begin{cases} \frac{x^{\alpha-1}e^{-\frac{x}{\theta}}}{\theta^\alpha \Gamma(\alpha)} & \text{for } x > 0 \\ 0 & \text{for } x = 0 \end{cases} \quad (5.4)$$

where $\alpha > 0$ is the shape, and $\theta > 0$ the scale parameter. The pdf of the generalized pareto (GP) distribution is defined via

$$g(x) = \begin{cases} \frac{1}{\sigma} \left(1 + \frac{\xi(x-\mu)}{\sigma}\right)^{-\frac{1}{\xi}-1} & \text{for } \xi \neq 0 \\ \frac{1}{\sigma} e^{-\frac{x-\mu}{\sigma}} & \text{for } \xi = 0 \end{cases} \quad (5.5)$$

with $\sigma > 0$ being the scale parameter and $\xi \in \mathbb{R}$ the shape parameter. μ is the location parameter.

Following Furrer and Katz, 2008, we define the hybrid gamma-GP pdf as

$$h(x) = \begin{cases} f(x) & \text{for } x \leq \mu \\ (1 - F(\mu)) g(x) & \text{for } x > \mu \end{cases}, \quad (5.6)$$

where $F(\mu)$ describes the cumulative gamma distribution function at the threshold μ . In our weather generator however, we first draw a random number from the gamma distribution and, if we are above the threshold, we draw another random number from the GP distribution. Thus, the frequency of precipitation events larger than μ is determined by the gamma distribution, but the actual amount of precipitation simulated when above the threshold μ is determined by the GP distribution (*ibid.*).

To determine the parameters of the hybrid distribution for precipitation, we started with the simple strategy by S. Geng et al., 1986. As above when calculating the Markov chain parameters, we created multi-year series for each of the parameterization stations for each month and extracted the days with precipitation. If a series contained more than 100 entries, we fit a gamma distribution using maximum likelihood to it in order to estimate the α and θ parameters.

Following *ibid.*, we then fit a regression line of the gamma scale parameter against the mean precipitation on wet days \bar{p}_d (see figure 5.4) and found the relationship

$$\theta = 1.262 \bar{p}_d. \quad (5.7)$$

As proposed by *ibid.*, we use this relationship in our model to estimate the scale parameter of the distribution. Using this approach, the gamma shape parameter α is a constant, given via

$$\alpha = \frac{\bar{p}_d}{\theta} = \frac{1}{1.262}. \quad (5.8)$$

The GP scale parameter σ on the other hand is calculated during the simulation following Neykov et al., 2014 via

$$\sigma = \frac{1 - F(\mu)}{f(\mu)}. \quad (5.9)$$

The other parameters of the GP distribution are obtained through a sensitivity analysis described in section 5.3.5.

Temperature

Following the standard WGEN methodology (Richardson, 1981) and S. Geng et al., 1986, daily temperature is determined through 2 processes: First, the wet/dry state of the day, and second the cross correlation (Equation 5.3.2).

In the weather generator, we know from the Markov chain (section 5.3.2), whether the current simulated day is a wet or dry day. Based upon the simple linear relationships

$$\begin{aligned} \bar{x}_{\text{wet}} &= c_{0,x,\text{wet}} + c_{1,x,\text{wet}} \cdot \bar{x} \\ \bar{x}_{\text{dry}} &= c_{0,x,\text{dry}} + c_{1,x,\text{dry}} \cdot \bar{x} \end{aligned} \quad (5.10)$$

we adjust the monthly mean \bar{x} of the variable $x \in \{T_{\min}, T_{\max}\}$.

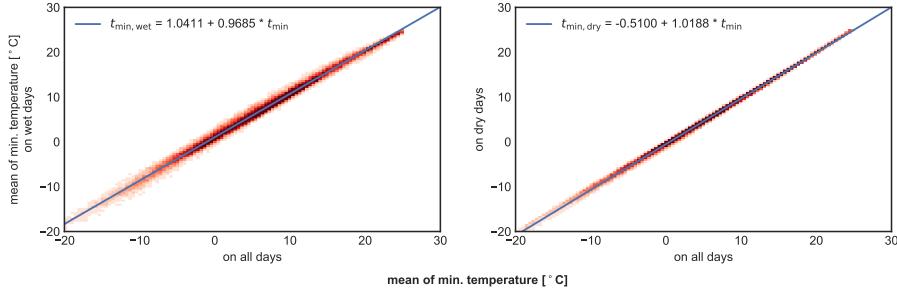


FIGURE 5.5: Correlation of minimum temperature on wet and dry days to the monthly mean. The y-axes show the mean minimum temperature on wet or dry days respectively, the blue line corresponds to the best fit line. Parameters of the fits are also shown in table 5.1.

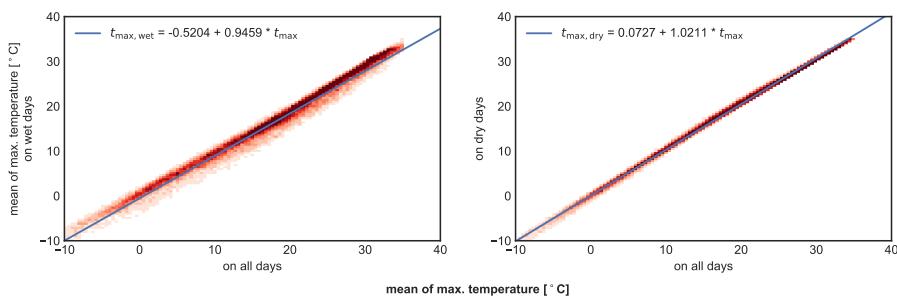


FIGURE 5.6: Correlation of maximum temperature on wet and dry days to the monthly mean. The y-axes show the mean maximum temperature on wet or dry days respectively, the blue line corresponds to the best fit line. Parameters of the fits are also shown in table 5.1.

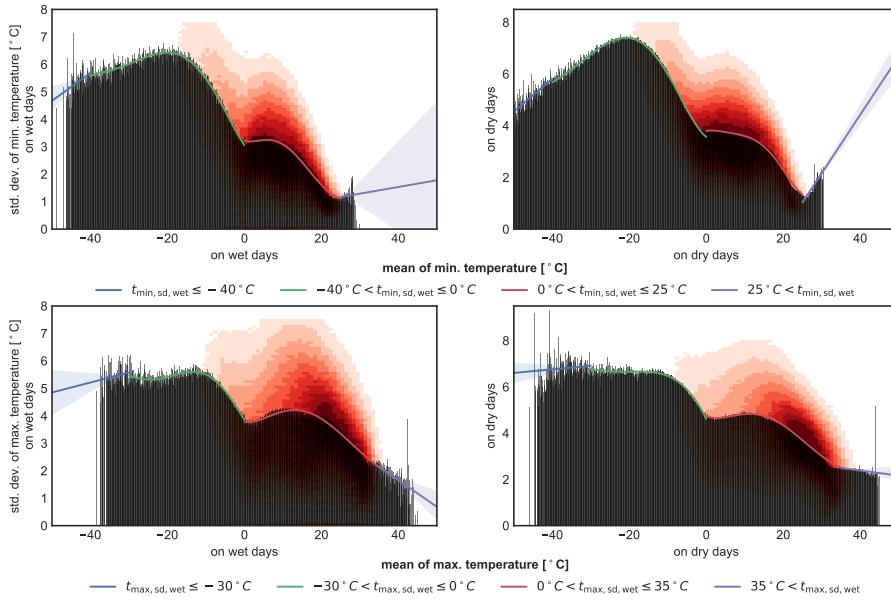


FIGURE 5.7: Correlation of standard deviation of the minimum and maximum temperature on wet and dry days to the monthly mean. The y-axes show the standard deviation, the x-axes the mean on wet or dry days respectively. The bars have a width of 0.1°C (the data accuracy) and indicate the mean standard deviation for a given mean minimum temperature in one month. The lines are fitted to these bars, where the green and red polynomials of order 5 are the use all the data below or above 0°C respectively and the blue and violet lines are a linear extrapolation of the data below -40°C (or -30°C for T_{\max}) or above 25°C (or 35°C) respectively. The red density plot in the background indicates the spread of the data. The bars and the density plot are based on the single month for each station (i.e. not the multi-year monthly series as for, e.g. mean temperature (figure 5.5 and 5.6)). Parameters of the fits are also shown in table 5.1.

TABLE 5.1: Fit results of temperature correlation for wet and dry days for figures 5.5, 5.6, 5.10 and 5.11. The coefficients c_0 to c_3 correspond to the coefficients used in equations (5.10) and (5.14).

plot	variable	R^2	c_0	c_1	c_2	c_3
5.6	$T_{\text{max,dry}}$	0.9969	0.0727	1.0211	0	0
5.6	$T_{\text{max,wet}}$	0.9752	-0.5204	0.9459	0	0
5.5	$T_{\text{min,dry}}$	0.9972	-0.5100	1.0188	0	0
5.5	$T_{\text{min,wet}}$	0.9840	1.0411	0.9685	0	0
5.11	$w_{\text{sd,dry}}$	0.4243	0	1.0860	-0.2407	0.0222
5.11	$w_{\text{sd,wet}}$	0.5003	0	0.8184	-0.1263	0.0093
5.10	w_{dry}	0.9930	0	0.9437	0	0
5.10	w_{wet}	0.9723	0	1.0937	0	0

To estimate the values of the parameters c_0 and c_1 in the above equations, we follow the same procedure as for the parameters of the Markov chain (section 5.3.2). We extracted the complete months for T_{min} and T_{max} from the GHCN-Daily dataset and created a multi-year series for each month and station. We then regressed the mean on wet and dry days separated against the overall mean of each month (Figures 5.5 and 5.6). Through this procedure, we estimate the parameters necessary for equations (5.10) (see table 5.1).

To estimate residual noise, we also need an estimate of the standard deviation of the variable (see Equation 5.3.2). Figure 5.7 shows the correlation between standard deviation on wet and dry days and the corresponding mean. The means of the standard deviations (black bars in figure 5.7) indicate a strong but non-linear relationship between the standard deviation and the corresponding mean. The correlation changes particularly at 0°C . We therefore use two different polynomials of order 5 for the values below and above the freezing point. Furthermore, to account for the sparse data below -40°C and above 25°C for minimum temperature (or -30°C and 35°C for maximum temperature), we use an extrapolation for the extremes as indicated by the blue and violet lines in figure 5.7. The formulae for the standard deviations σ of minimum and maximum temperature are therefore a combination of 4 polynomials:

$$\sigma_{T_{\text{min}},\text{wet/dry}} = \begin{cases} p_1(\bar{T}_{\text{min,wet/dry}}), & \text{for } \bar{T}_{\text{min,wet/dry}} \leq -40^\circ \text{C} \\ p_5(\bar{T}_{\text{min,wet/dry}}), & \text{for } -40^\circ \text{C} < \bar{T}_{\text{min,wet/dry}} \leq 0^\circ \text{C} \\ p_5(\bar{T}_{\text{min,wet/dry}}), & \text{for } 0^\circ \text{C} < \bar{T}_{\text{min,wet/dry}} \leq 25^\circ \text{C} \\ p_1(\bar{T}_{\text{min,wet/dry}}), & \text{for } 25^\circ \text{C} < \bar{T}_{\text{min,wet/dry}} \end{cases}$$

$$\sigma_{T_{\text{max}},\text{wet/dry}} = \begin{cases} p_1(\bar{T}_{\text{max,wet/dry}}), & \text{for } \bar{T}_{\text{max,wet/dry}} \leq -30^\circ \text{C} \\ p_5(\bar{T}_{\text{max,wet/dry}}), & \text{for } -30^\circ \text{C} < \bar{T}_{\text{max,wet/dry}} \leq 0^\circ \text{C} \\ p_5(\bar{T}_{\text{max,wet/dry}}), & \text{for } 0^\circ \text{C} < \bar{T}_{\text{max,wet/dry}} \leq 35^\circ \text{C} \\ p_1(\bar{T}_{\text{max,wet/dry}}), & \text{for } 35^\circ \text{C} < \bar{T}_{\text{max,wet/dry}} \end{cases}. \quad (5.11)$$

p_1 in eq. (5.11) denotes a polynomial of order 1, p_5 a polynomial of order 5. The coefficients of the different polynomials are shown in table 5.2.

These coefficients are based on the means of the standard deviation (black bars in figure 5.7). We chose this procedure to give the same weight to all temperatures.

TABLE 5.2: Fit results of the correlation of temperature standard deviation with the corresponding mean on wet/dry days for figure 5.7.
 The underlying equations are shown in equation (5.11).

variable	interval	R^2	c_0	c_1	c_2	c_3	c_4	c_5
$T_{\max, \text{sd}, \text{dry}}$	($-\infty$, -30]	0.0125	7.3746	0.0154	0	0	0	0
	(-30, 0.0]	0.6721	4.6170	-0.3387	-0.0188	-0.0003	0.000003	0.0000001
	(0.0, 35]	0.9744	4.7455	-0.0761	0.0189	-0.0013	0.00003	-0.0000002
	(35, ∞)	0.0390	3.2554	-0.0218	0	0	0	0
$T_{\max, \text{sd}, \text{wet}}$	($-\infty$, -30]	0.0366	6.6720	0.0364	0	0	0	0
	(-30, 0.0]	0.7362	3.8601	-0.2186	0.0039	0.0015	0.00006	0.0000007
	(0.0, 35]	0.9508	3.7919	-0.0313	0.0161	-0.0012	0.00003	-0.0000002
	(35, ∞)	0.2530	5.5529	-0.0973	0	0	0	0
$T_{\min, \text{sd}, \text{dry}}$	($-\infty$, -40]	0.6006	10.8990	0.1271	0	0	0	0
	(-40, 0.0]	0.9509	3.5676	-0.1154	0.0282	0.0020	0.00004	0.0000003
	(0.0, 25]	0.9825	3.7941	0.0330	-0.0150	0.0019	-0.0001	0.000002
	(25, ∞)	0.7784	-4.6194	0.2261	0	0	0	0
$T_{\min, \text{sd}, \text{wet}}$	($-\infty$, -40]	0.1661	9.7272	0.1011	0	0	0	0
	(-40, 0.0]	0.9285	3.0550	-0.2116	0.0137	0.0014	0.00004	0.0000003
	(0.0, 25]	0.9633	3.2187	-0.0451	0.0209	-0.0026	0.00010	-0.000001
	(25, ∞)	0.0089	0.5571	0.0244	0	0	0	0

Otherwise the fit would be dominated by the temperature values around the freezing points.

Cloud fraction

Monthly mean cloud fraction is disaggregated, as for temperature, using the standard WGEN procedure of adding statistical noise to a wet- or dry-day mean and accounting for cross-correlation among the different weather variables. For the parameterization of the cloud fraction equations, we used the EECRA dataset. The original dataset contains eight measurements per day of the total cloud cover in

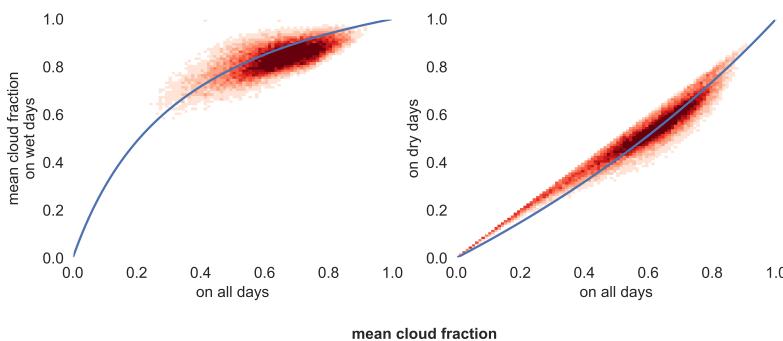


FIGURE 5.8: Correlation of cloud fraction on wet and dry days to the monthly mean. The y-axes show the mean cloud fraction on wet or dry days respectively, the blue line corresponds to the best fit line. Parameters of the fits are also shown in table 5.3.

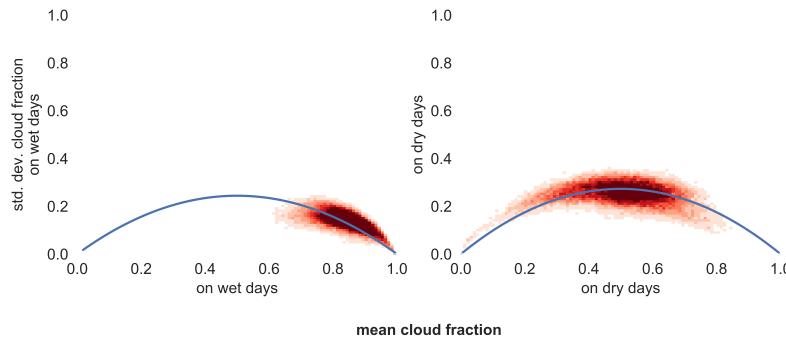


FIGURE 5.9: Correlation of standard deviation of the cloud fraction on wet and dry days to the corresponding monthly mean. The y-axes show the standard deviation, the x-axes the mean on wet or dry days respectively. The blue line corresponds to the best fit line. Parameters of the fits are also shown in table 5.3.

TABLE 5.3: Fit results of cloud correlation for wet and dry days for figure 5.8

plot	variable	a	std. err. of a	R^2
5.8	c_{dry}	0.4302	0.0013	0.8745
5.8	c_{wet}	-0.7376	0.0006	0.3881
5.9	$c_{\text{sd,dry}}$	1.0448	0.0004	0.2803
5.9	$c_{\text{sd,wet}}$	0.9881	0.0006	0.0802

units of octas, i.e., values ranging from 0 (clear sky) to 8 (overcast). Hence, to calculate the daily cloud fraction, those values were averaged and divided by 8 to produce a daily mean.

To adjust the monthly mean depending on the wet/dry state of the day, we could not use a simple linear relationship as we used for temperature because cloud fraction is bounded by a lower limit 0 and an upper limit of 1. Furthermore, we observed that cloud cover on wet days is usually greater or equal to the monthly mean cloud cover, whereas the cloud cover on dry days is usually less or equal to the monthly mean cloud cover. This results in a concave curve for the wet case and a convex curve for dry days. We used a qualitative graphical analysis to develop "best guess" equations that had the desired shape and propose the following formulae for the regression linking cloud cover on wet or dry days to the overall mean:

$$\begin{aligned}\bar{c}_{\text{wet}} &= \frac{-a_{c,\text{wet}} - 1}{a_{c,\text{wet}}^2 \cdot \bar{c} - a_{c,\text{wet}}^2 - a_{c,\text{wet}}} - \frac{1}{a_{c,\text{wet}}} \\ \bar{c}_{\text{dry}} &= \frac{-a_{c,\text{dry}} - 1}{a_{c,\text{dry}}^2 \cdot \bar{c} - a_{c,\text{dry}}^2 - a_{c,\text{dry}}} - \frac{1}{a_{c,\text{dry}}}\end{aligned}\quad (5.12)$$

with $a_{c,\text{wet}} < 0$ and $a_{c,\text{dry}} > 0$.

The standard deviation of cloud cover fraction becomes 0 when the mean monthly cloud fraction reaches both the minimum or maximum limits of 0 and 1. Hence, for $c_{\text{sd,dry}}$ and $c_{\text{sd,wet}}$ we have an concave parabola with the formula

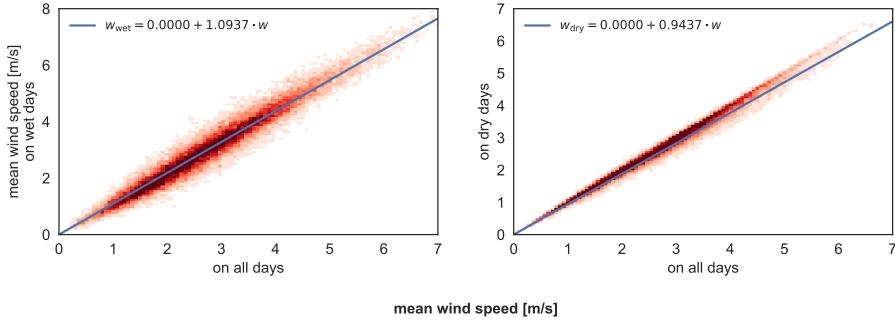


FIGURE 5.10: Correlation of wind speed on wet and dry days to the monthly mean. The y-axes show the mean cloud fraction on wet or dry days respectively, the blue line corresponds to the best fit line. Parameters of the fits are also shown in table 5.1.

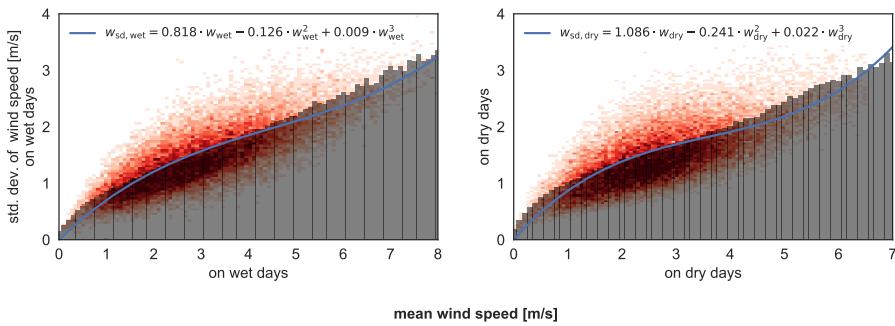


FIGURE 5.11: Correlation of standard deviation of wind speed on wet and dry days to the corresponding monthly mean. The y-axes show the standard deviation, the x-axes the mean on wet or dry days respectively. The blue line corresponds to the best fit line, a third order polynomial to the underlying red density plot. The black bars have a width of 0.1 m s^{-1} , the accuracy of the input data, and indicate the mean standard deviations for the given interval range. Parameters of the fits are also shown in table 5.1.

$$\begin{aligned}\sigma_{c,wet} &= a_{c,wet}^2 \cdot \bar{c}_{wet} \cdot (1 - \bar{c}_{wet}) \\ \sigma_{c,dry} &= a_{c,dry}^2 \cdot \bar{c}_{dry} \cdot (1 - \bar{c}_{dry})\end{aligned}\quad (5.13)$$

with $a_{c,wet}, a_{c,dry} \geq 0$. Results of the fits can be seen in figure 5.8, 5.9 and the parameters in table 5.3.

Wind speed

The parameterization of the mean wind speed is based upon the same linear equation (5.10) as temperature. For the standard deviation however, we use a third-order polynomial given that is forced through the origin, given via

$$\begin{aligned}\sigma_{w,wet}(\bar{w}_{wet}) &= c_{1,w,wet} \bar{w}_{wet} + c_{2,w,wet} \bar{w}_{wet}^2 + c_{3,w,wet} \bar{w}_{wet}^3 \\ \sigma_{w,dry}(\bar{w}_{dry}) &= c_{1,w,dry} \bar{w}_{dry} + c_{2,w,dry} \bar{w}_{dry}^2 + c_{3,w,dry} \bar{w}_{dry}^3.\end{aligned}\quad (5.14)$$

This better resolves the complex behavior close to 0 m s^{-1} compared to a linear fit. The plots are shown in the figures 5.10 and 5.11 and the parameters for the fits are shown in table 5.1.

Cross correlation

Following Richardson, 1981 we use cross correlation to add additional residual noise to the simulated meteorological variables, which provides more realism in the daily weather result. This methodology, based on Matalas, 1967 preserves the serial and the cross correlation between the simulated variables. It implies that the serial correlation of each variable may be described by a first-order linear autoregressive model

Given the cross correlation matrix $M_0 \in \mathbb{R}^4 \times \mathbb{R}^4$ and the lag-1 correlation matrix $M_1 \in \mathbb{R}^4 \times \mathbb{R}^4$, we calculate

$$A = M_1 M_0^{-1} \quad BB^T = M_0 - M_1 M_0^{-1} M_1^T. \quad (5.15)$$

The matrices A, B, M_0 and M_1 are calculated using the stations from the EECRA database in figure 5.2. The results are

$$M_0 = \begin{pmatrix} 1. & 0.565 & 0.041 & 0.035 \\ 0.565 & 1. & -0.089 & -0.043 \\ 0.041 & -0.089 & 1. & 0.114 \\ 0.035 & -0.043 & 0.114 & 1. \end{pmatrix} \quad M_1 = \begin{pmatrix} 0.933 & 0.55 & 0.016 & 0.03 \\ 0.557 & 0.417 & -0.066 & -0.043 \\ 0.004 & -0.095 & 0.599 & 0.093 \\ 0.011 & -0.063 & 0.061 & 0.672 \end{pmatrix}. \quad (5.16)$$

leading to

$$A = \begin{pmatrix} 0.916 & 0.031 & -0.018 & 0.001 \\ 0.485 & 0.135 & -0.069 & -0.047 \\ 0.004 & -0.043 & 0.592 & 0.023 \\ 0.012 & -0.043 & -0.02 & 0.672 \end{pmatrix} \quad B = \begin{pmatrix} 0.358 & 0. & 0. & 0. \\ 0.112 & 0.809 & 0. & 0. \\ 0.142 & -0.06 & 0.785 & 0. \\ 0.077 & -0.016 & 0.061 & 0.733 \end{pmatrix}. \quad (5.17)$$

The columns and rows in the two matrices correspond to min. and max. temperature, cloud fraction and square root of wind speed, respectively.

In the weather generator, the variables T_{\min}, T_{\max}, c and w are then calculated using a combination of residual noise χ_i (where i denotes the current simulated day) and the mean of the variables. χ_i is determined by the other variables and the previous day using A and B from above (Matalas, 1967; Richardson, 1981). Hence, χ_i is given via

$$\chi_i = (\chi_{T_{\min}} \quad \chi_{T_{\max}} \quad \chi_c \quad \chi_w) = A \chi_{i-1} + B \epsilon \in \mathbb{R}^4. \quad (5.18)$$

The daily values for the variables are then calculated via

$$T_{\min,i} = \chi_{T_{\min}} \cdot \sigma_{T_{\min}, \text{wet/dry}} + \bar{T}_{\min, \text{wet/dry}} \quad c_i = \chi_c \cdot \sigma_{c, \text{wet/dry}} + \bar{c}_{\text{wet/dry}} \quad (5.19)$$

$$T_{\max,i} = \chi_{T_{\max}} \cdot \sigma_{T_{\max}, \text{wet/dry}} + \bar{T}_{\max, \text{wet/dry}} \quad w_i = \left(\chi_w \cdot \sqrt{\sigma_{w, \text{wet/dry}}} + \sqrt{\bar{w}_{\text{wet/dry}}} \right)^2 \quad (5.20)$$

with $\sigma_{T_{\min}, \text{wet/dry}}, \sigma_{T_{\max}, \text{wet/dry}}$ from eq. (5.11), $\sigma_{c, \text{wet/dry}}$ from eq. (5.13), $\sigma_{w, \text{wet/dry}}$ from eq. (5.14), $\bar{T}_{\min, \text{wet/dry}}, \bar{T}_{\max, \text{wet/dry}}, \bar{w}_{\text{wet/dry}}$ from eq. (5.10) and $\bar{c}_{\text{wet/dry}}$ from eq. (5.12).

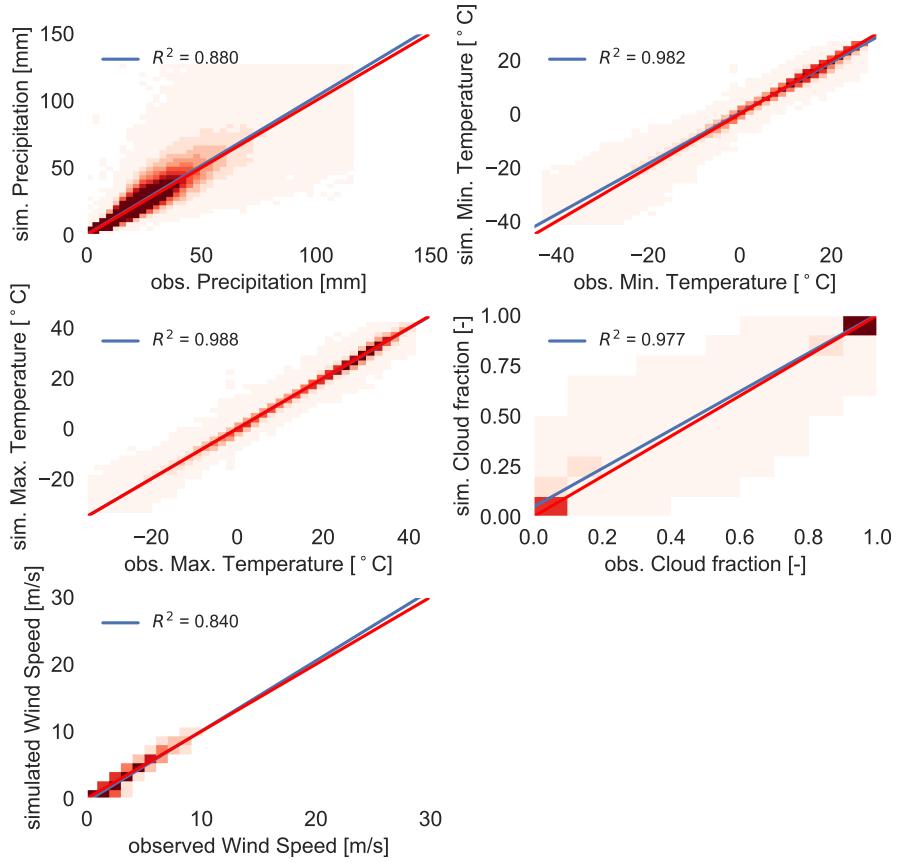


FIGURE 5.12: QQ-plots for all variables with all quantiles (1, 5, 10, 25, 50, 75, 90, 95 and 99) for $\mu = 5.0 \text{ mm mm}$, $\xi = 1.5$. The blue lines are linear regression from simulation to observation. The red line shows the ideal fit (the identity line). Blue shaded areas represent the 95% confidence interval. The plots compares the simulated quantile from the list above of one year of one station to the corresponding observed quantile of the same year and station. The plot for wind speed underwent used the bias correction from subsection 5.3.4.

Since this procedure always requires the residuals from the previous day, χ_{i-1} , we initialize χ_0 with 0, simulate the month and then simulate it again.

Note that, through the entire procedure, wind speed is subject to a square-root transformation (also when calculating M_0 and M_1) to account for the fact that it is not normally distributed.

5.3.3 Model Evaluation

To evaluate GWGEN, we started with the daily meteorology at the evaluation stations described above and calculated monthly summaries. We used this monthly data to drive the model and simulate daily meteorology. The resulting daily series now has the same length as the observed meteorology from the GHCN and EECRA database. Because we cannot expect the weather generator to reproduce the weather exactly as observed, for example the number of rainy days in a month may be the same as observed but they may not occur in precisely the same order, our evaluation is restricted to comparing the statistical properties of the input observed versus the output simulated daily meteorology.

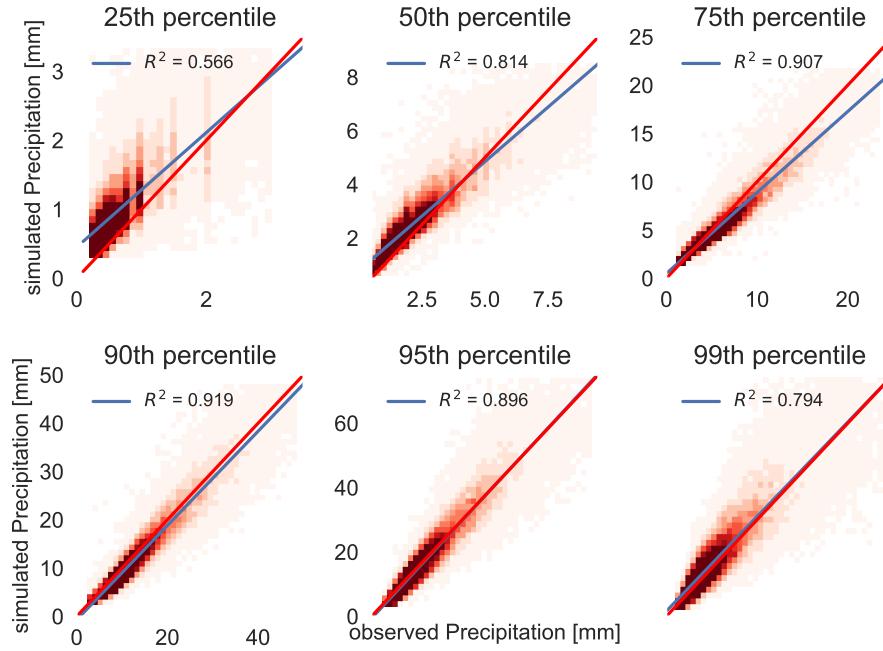


FIGURE 5.13: QQ-plot for different quantiles for precipitation for $\mu = 5.0\text{mm}$, $\zeta = 1.5$. The blue lines are linear regression from simulation to observation. The red line shows the ideal fit (the identity line). Blue shaded areas represent the 95% confidence interval. The plots compare the simulated quantile of one year of one station to the corresponding observed quantile of the same year and station.

Figure 5.12 shows the comparison of simulated versus observed values for each of the five meteorological variables handled by GWGEN. For temperature, wind, and cloud fraction, the model does an excellent job of downscaling monthly input to daily resolution¹. The comparison between precipitation amounts looks good when considering all of the data, however a closer look into the results (Fig. 5.13) shows that while the higher precipitation percentiles are well captured using the hybrid Gamma-GP distribution, the lower percentiles show somewhat worse results. This observation of poor performance for very low values also holds true for wind speed (not shown here). The lower values of the two variables, however, are very close to the precision of the observation (0.1 mm for precipitation and 0.1 m s^{-1} for wind speed). Very small precipitation amounts and low wind speeds are also less biophysically and ecologically important compared to the higher percentiles. We therefore consider the results of the evaluation largely acceptable.

In table 5.4 we also compare the simulated versus the observed frequencies. For very light rain ($<=1\text{mm}$), light rain (1-10mm), heavy rain (10-20mm) and very heavy rain ($>20\text{mm}$). As we can see, our model underestimates the occurrence of very light rain events (28.6% instead of 36.4%) and overestimates the light rain events (58.3% instead of 48.6%) but generally performs much better than GCMs (Dai, 2006; Sun et al., 2006), especially when it comes to the heavy rain events.

TABLE 5.4: Simulated and observed precipitation frequencies for certain ranges. The frequency is defined as the number of precipitation occurrences in the specified range, divided by the total number of precipitation occurrences.

Precip. range [mm]	Simulated	Observed
(0, 1]	0.285688	0.364014
(1, 10]	0.583330	0.486415
(10, 20]	0.074063	0.090178
(20, ∞]	0.056920	0.059392

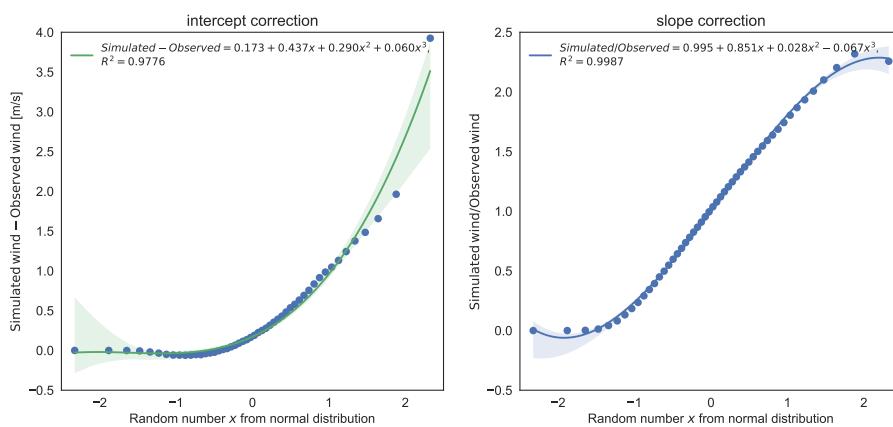


FIGURE 5.14: Basis for the wind bias correction. For the left plot, each data point corresponds to the difference of a simulated percentile to the observed percentile. For the right plot (wind speed), each data point corresponds to the fraction of simulated to the observed wind speed for a given percentile. The random number on the x-axis represents the residual value from a normal distribution centered at 0 with standard deviation of unity, as it is used in the cross correlation approach (Richardson, 1981).

5.3.4 Bias correction

After evaluating the results of GWGEN for wind speed for the different quantiles (see previous subsection 5.3.3) we found a strong, systematic bias between the simulated and the observed values. This observation led us to adopt a further measure to improve the quality of the model output by implementing a quantile-based bias correction.

We use an empirical distribution correction approach (quantile-mapping) (Lafon et al., 2012) to a posteriori correct the simulated data. In the quantile evaluation (previous subsection 5.3.3) we saw that the simulated wind speed is a linear function of the observed wind speed, i.e. $w_{sim} = \text{intercept} + \text{slope} \cdot w_{obs}$ (best fit line in figure 5.12). Therefore, we use two steps here, one is for the difference between simulation and observation (ideally 0), the other one is the fraction of observation and simulation (ideally 1). The first one corresponds to the intercept with the y-axis in figure 5.12, the second one to the slope of the best fit line. The analysis is based on every second percentile between 1 and 100 (i.e. 1, 3, 5, ...) and mapped to its corresponding random number $u \in \mathbb{R}$ from a normal distribution as it is used for the cross correlation in the weather generator (section 5.3.2, x-axis in figure 5.14 and Richardson, 1981).

Regarding the intercept (fig. 5.14, left) we see that it strongly follows an exponential function given through

$$f_{exp}(u) = e^{au+b}, \quad a, b, u \in \mathbb{R}. \quad (5.21)$$

The slope (fig. 5.14, right) on the other hand can be described by a simple third-order polynomial given by

$$p3(u) = c_0 + c_1 u + c_2 u^2 + c_3 u^3, \quad c_0, c_1, c_2, c_3, u \in \mathbb{R} \quad (5.22)$$

Hence, given the best fit lines in figure 5.14, the simulated wind speed is corrected via

$$w'_{sim} = \frac{w_{sim} - f_{exp}(u)}{p3(u)} \quad (5.23)$$

with $a = 1.1582, b = -1.3359, c_0 = 0.9954, c_1 = 0.8508, c_2 = 0.0278, c_3 = -0.0671$.

5.3.5 Sensitivity analysis

The Generalized-Pareto part of the hybrid Gamma-GP distribution, which we used to simulate precipitation amount, has two parameters: the GP shape, and the threshold parameter. Unlike the gamma parameters, we were unable to relate these GP parameters to any of the monthly summary data we use as input to GWGEN. Hence, we decided to set fixed values for these parameters, and determine them through a sensitivity analysis.

To select the "best" values of the GP parameters, we compared simulated with observed precipitation amounts, running GWGEN with a wide range of realistic parameter values. To quantitatively assess the model performance, we used two metrics: 1) direct comparison of the quantiles (see previous section), and 2) a Kolmogorov-Smirnov (KS) test that evaluates whether two data samples come from significantly different distributions. Our criteria were

1. The R^2 correlation coefficient between simulated and observed quantiles

¹Note that the plot for wind speed has been bias corrected using the approach in subsection 5.3.4.

2. The fraction $\frac{\text{simulated precipitation}}{\text{observed precipitation}}$ from the slopes in figure 5.13 and it's deviation from unity
3. the fraction of simulated (station specific) years that are significantly different (KS test) from the observation
4. The mean of the above values

We tried two different approaches to select the gamma-GP crossover threshold: first we tried a fixed crossover point, second we used a quantile-based crossover point. For the latter, the model chooses to use the GP distribution if the quantile of the random number drawn from the gamma distribution is above a certain quantile threshold. This introduces a flexible crossover point in our hybrid distribution which, however, did not improve the results significantly. We therefore show here only the results using the fixed crossover point.

The values of the crossover point for our sensitivity analysis were 2, 2.5, 3, 4 and from 5 to 20 in steps of 2.5 and 20 to 100 in steps of 5. Furthermore we varied the GP shape parameter from 0.1 to 3 in steps of 0.1 (810 experiments in total). The results of this sensitivity analysis are shown in the supplementary material, figure 5.15.

In general we found that the three criteria 1, 2 and 3 could not be optimized all together at the same time. The R^2 is best for high thresholds and low GP shape parameters, the slope is best for low to intermediate thresholds and a low GP shape and the KS statistic is best for low threshold and intermediate GP shape parameters.

However, R^2 did not vary that much (from 0.68 to 0.74) and from a visual evaluation of the corresponding quantile plots we saw that the higher quantiles (>90) were much better represented for a better KS result. Hence we chose to follow the KS test criteria, which is also the strictest of our evaluation methods but again compared the different quantile plots to get good results for the higher quantiles. Finally, we chose a threshold of 5 mm and a GP shape parameter of 1.5. For this setting, 81.7% of the simulated years do not show a significant difference compared to the observation, the mean R^2 of the plots in figure 5.13 is 0.81 and the mean deviation of the slope from unity is 0.10 and for the upper quantiles (90 to 100), 0.017.

Nevertheless, in total the results seem to be fairly independent of the two parameters since even the amount of years without significant differences vary from 73% to only 83%. It is however better than the gamma distribution alone which still has 78.6% of station years not differing significantly but with a slope deviation from unity for the upper quantiles of 0.16. Thus using the hybrid Gamma-GP distribution improves the simulation of high-amount precipitation events by roughly factor 10 compared to a standard Gamma approach.

5.4 Limitations

As demonstrated above, GWGEN successfully downscale monthly to daily meteorology with good correlation and low bias when compared to observations. However, there are a few limitations of the model as currently described that should be noted. Importantly, this version of GWGEN neither downscale all conceivable meteorological variables, nor does it provide a mechanism for generating daily meteorological timeseries across multiple points that are spatially autocorrelated. Concerning the former point, while GWGEN simulates daily precipitation, temperature, cloud cover, and windspeed, it does not currently handle other variables that might be important in land surface modeling, such as humidity or wind direction. On the

latter point, the lack of explicit simulation of spatial autocorrelation may make GWGEN unsuitable for certain applications, e.g., regional high-resolution hydrological modeling in small catchments (< ca. 2500 km²), where having the capability to simulate flood and other extremes is important. This is because the weather generator could, e.g., simulate rainfall on different days in different parts of the catchment, where in reality storm events would be highly autocorrelated in space and controlled by mesoscale meteorological conditions.

5.5 Discussion and Outlook

GWGEN successfully downscals monthly to daily meteorology, for any point on the globe, in any climate, in any season, and in any time in recent earth history and into the near future (e.g., next century). It extends the original Richardson-type weather generators to simulate wind speed along with precipitation, temperature, and cloud cover. The model requires only monthly values of the meteorological variables to be downscaled, and does not rely on any other spatial information, e.g., whether or not the location is in the tropics.

In general, the results of our downscaled meteorology are excellent, with all simulated variables showing both very high correlation and limited bias when compared to observations. We improved the simulation of daily precipitation amount by replacing the Gamma distribution used in the original Richardson-type weather generators with a hybrid Gamma-GP distribution, which results in the improved simulation of heavy precipitation events. The GP distribution is based upon a globally fixed shape and location parameter, which may be an oversimplification, but is still ten times more accurate than traditional methods that used Gamma alone. Our extensive sensitivity analysis to determine the best coefficients for the shape and location parameters of the GP distribution suggest that further improvements might come through correlating the GP parameters to geographic region and/or seasonality (Maraun et al., 2009; Rust et al., 2009) or by introducing a dynamical location parameter (Frigessi et al., 2002). Finally, we introduced a step to correct for systematic bias in the downscaling of temperature and wind speed.

Despite the limitations noted above, GWGEN will be useful in a wide range of applications, from global vegetation and crop modeling, to large-scale hydrologic analyses, to understanding animal behavior, to forecasting of fire, insect outbreaks, and other ecosystem disturbances. GWGEN may even be envisaged as a potential replacement for very large and cumbersome gridded datasets of high-temporal resolution meteorology such as CRUNCEP (Viovy and Ciais, 2016), especially for models that use meteorological forcing at a daily timestep. The weather generator is particularly suited for the incorporation into models that run on a spatial grid, for example, GWGEN can readily be incorporated into existing DGVMs such as LPJ-LMfire (Pfeiffer et al., 2013) or LPJ-ML (Bondeau et al., 2007) that already rely on a weather generator to provide daily meteorology for certain processes.

While GWGEN does not handle spatial autocorrelation, in most DGVMs there is no lateral connection between gridcells, and therefore an explicit representation of spatial autocorrelation in the driving daily meteorological data would have no effect on the model output. We further note that if the monthly data used to drive the model are spatially autocorrelated — this would be the case when using gridded climatology for example — then the result of the weather generator will also preserve this autocorrelation, at least when the model results are analyzed on monthly or longer timescales.

The limitations present in this version of GWGEN could be addressed in future versions. Methods for simultaneous multisite weather generation exist (D. S. Wilks, 1998, 1999b,c) and could be adapted to GWGEN. However, even simpler methods to approximate spatial autocorrelation could be possible. Running GWGEN with gridded monthly meteorology — this is the primary application we foresee for the current version of the model — means that the input variables are already highly correlated in space, i.e., the monthly climate in one gridcell generally closely resembles neighboring cells, outside of complex terrain containing sharp, monotonic climate gradients, e.g., rain shadows. Thus, one simple way of achieving a measure of spatial autocorrelation in GWGEN would be to impose a spatial autocorrelation field on the sequence of random numbers used to impose stochastic noise in the downscaling functions. If the random number sequence is similar between gridcells, then, e.g., rain is likely to fall on the same day, given that the transition probabilities will likely also be similar. Over moderate distances, e.g., <50's of km, it might even be sufficient to use the same random seed across all gridcells in a neighborhood. This would have the effect of producing strongly autocorrelated daily meteorology in space, with the only variations being imposed by the underlying input monthly climatology.

Furthermore, it would be straightforward to include additional meteorological variables in the model framework, handling, e.g., humidity in the same way that temperatures, cloud cover, and wind speed are disaggregated. Other variables, such as pressure and wind direction, might be more difficult using the basic GWGEN structure because of the importance of autocorrelation, particularly at high spatial resolution, and might benefit from a different approach towards weather generation. Finally, GWGEN only downscales meteorology from monthly to daily values; for models that require an even shorter timestep, e.g., 6-hourly, some extension of the model functionality would be required. For certain variables, e.g., temperatures, sub-daily downscaling could be easily implemented (Cesaraccio et al., 2001), for other variables, such as precipitation, a large literature on downscaling methods exists (e.g. Bennett et al., 2016), and global datasets of hourly meteorology for model calibration are available (e.g., the Integrated Surface Database, Smith et al., 2011).

5.6 Conclusions

Compiling a global database of daily precipitation, temperature, cloud cover, and wind speed measurements, we explored the relationship between daily meteorology and monthly summaries first described in the context of weather downscaling by Shu Geng and Auburn, 1987. Our analysis of more than 50 million individual records showed that daily-to-monthly relationships are relatively stable in space and time, and constant across a very wide range of stations from all latitudes and climate zones. With the resulting relationships, we parameterized a WGEN/SIMMETEO-type weather generator, with the intention of creating a generic scheme that could be applied anywhere over the earth's land surface for the past, present, and (near) future.

5.7 Code availability

GWGEN, is open source software, and the code, utility programs for parameterization, evaluation and manipulating the raw weather station data, and complete documentation are available at (Sommer and Jed O. Kaplan, 2017). The original

weather station database can be made available upon request to the authors or downloaded from Hahn and Warren, 1999 and Menne et al., 2012b. The weather generator module is programmed in FORTRAN, the parameterization, evaluation and other supplementary tools are written in Python mainly using the numerical python libraries numpy and scipy (E. Jones et al., 2001), statsmodels (Seabold and Perktold, 2010), as well as matplotlib (Hunter, 2007) and psyplot (Sommer, 2017) for the visualization. Detailed installation instructions can be found in the user manual: <https://arve-research.github.io/gwgen/>.

5.A Supplementary material

5.A.1 Sensitivity analysis

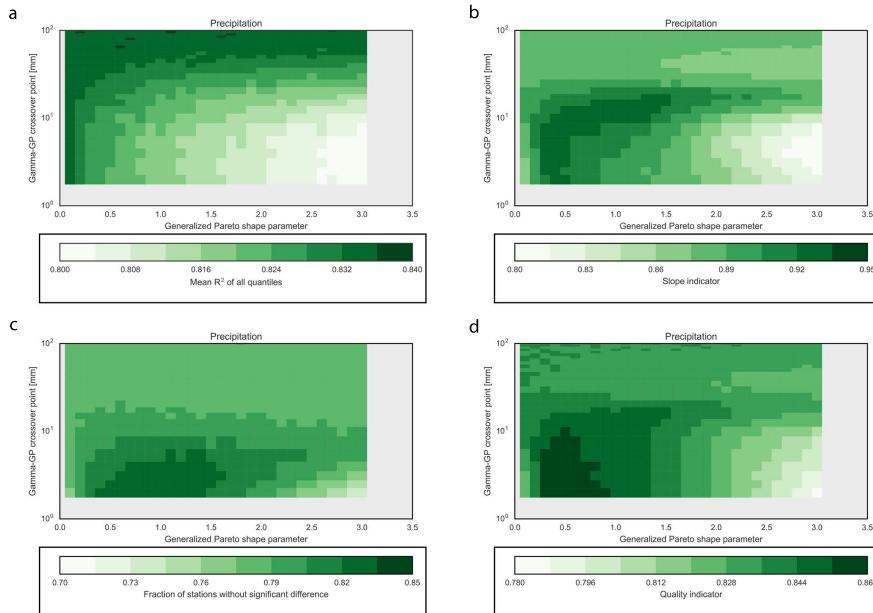


FIGURE 5.15: Results of the sensitivity analysis for the (a) correlation coefficient R^2 , (b) deviation from a slope of unity, (c) the fraction of significant different station years, (d) the mean of (a) - (c). For the plots in (a) and (b) we used the means of the 25th, 50th, 75th, 90th, 95th and 99th percentiles. In general, 1 (dark green) is best, 0 (white) is worst. The dark red fields indicate experiments that failed because of a too low threshold and too high GP shape parameter. Note the logarithmic scale on the y-axis.

Author contributions. JOK conceived the model and analyses, wrote the prototype code and performed preliminary analyses, PS developed and documented the final version of the code (including parameterization and evaluation), performed all of the final analyses, and created the graphical output. Both authors contributed to the writing of the manuscript

Acknowledgements. This work was supported by the European Research Council (COEVOLVE, 313797) and the Swiss National Science Foundation (ACACIA, CR10I2_146314). We thank Shawn Koppenhoefer for assistance compiling and querying the weather databases and Alexis Berne and Grégoire Mariéthoz for helpful suggestions on the analyses. We are grateful to NOAA NCDC and the University of Washington for providing free of charge the GHCN-Daily and EECRA databases, respectively.

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Chapter 6

A model analysis on the stability of northern hemispheric teleconnections

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Chapter 7

Conclusions

- New tools that have been developed
- Quality standards of the tools
- Further development and potential usage

Appendices

Todo list

1: Add reference.	1
2: Add reference.	1
3: Add reference. https://pangaea.de/	1
4: Add reference. EMPD paper	1
5: Add reference. ICON	1
6: Add reference. POLNET-gridding paper	1
7: Add reference.	2
8: Add reference.	2
9: Add reference. cite World bank report?	2
10: Add reference.	2
11: Add reference. check these references! taken from Achilles PhD thesis, there might be better ones	2
12: Add reference. Check these	2
13: Add reference. check Walker et al., 2009	2
14: Add some background on the Holocene. How did it change (global mean temperature estimate?), how was the insolation? CO ₂ effects, impact of the ice sheets during the early holocene, changes in altitude, large-scale atmospheric circulation, human influences.	2
15: Add reference. PMIP paper	2
16: Add reference.	3
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19: Add reference.	3
20: Add reference.	3
21: Add reference.	3
22: Add reference.	3
23: Add reference.	3
24: Add reference. Don't know about H. J. B. Birks and H. H. Birks, 1980, took it from Manus review paper...	3
25: Add reference. Manus review paper	3
26: Add reference. Don't know about Wodehouse, 1935, took it from Manus review paper...	3
27: Add reference. cite some MAT, WAPLS, Bayesian, etc. papers	3
28: Add reference. add more..., Climate12K	3
29: Add reference. cite some MAT papers	3
30: Add reference. that North-US/South-US discrepancy...	3
31: Add reference.	4
32: Add reference. cite some open-data publications	4
33: Add reference. add more?	5
Figure: Visualize multiple grids on the same map, e.g. by using the grid spec- ifications from Treut et al., 2007	6
34: Add reference.	6

■ Look into Dasgupta et al., 2016	7
■ 35: Add reference.	7
■ 36: Add reference.	7
■ 37: Add reference. jupyter qtconsole	7
■ Need to write chapter 2	23
■ Need to write chapter 3	25
■ Need to write chapter 4	27
■ Need to write chapter 6	63
■ Need to write chapter A	71
■ Need to write chapter C	75

Appendix A

Computing climate-smart urban land use with the Integrated Urban Complexity model (IUCm 1.0)

Need to write chapter A

Appendix B

Publications and Conference contributions

B.0.1 Peer-reviewed

- Cremades, R. and P. S. Sommer (2019). "Computing climate-smart urban land use with the Integrated Urban Complexity model (IUCm 1.0)". In: *Geoscientific Model Development* 12.1, pp. 525–539. DOI: [10.5194/gmd-12-525-2019](https://doi.org/10.5194/gmd-12-525-2019). URL: <https://www.geosci-model-dev.net/12/525/2019/>.
- Sommer, Philipp, Dilan Rech, Manuel Chevalier, and Basil Davis (2019). "stradielize: Digitizing stratigraphic diagrams". In: *Journal of Open Source Software* 4.34, p. 1216. DOI: [10.21105/joss.01216](https://doi.org/10.21105/joss.01216). URL: <https://doi.org/10.21105/joss.01216>.
- Weitzel, Nils, Sebastian Wagner, Jesper Sjolte, Marlene Klockmann, Oliver Bothe, Heather Andres, Lev Tarasov, Kira Rehfeld, Eduardo Zorita, Martin Widmann, Philipp S. Sommer, Gerd Schädler, Patrick Ludwig, Florian Kapp, Lukas Jonkers, Javier García-Pintado, Florian Fuhrmann, Andrew Dolman, Anne Dallmeyer, and Tim Brücher (2018). "Diving into the past – A paleo data-model comparison workshop on the Late Glacial and Holocene". In: *Bulletin of the American Meteorological Society*. DOI: [10.1175/bams-d-18-0169.1](https://doi.org/10.1175/bams-d-18-0169.1).
- Sommer, Philipp S (2017). "The psyplot interactive visualization framework". In: *The Journal of Open Source Software* 2.16. DOI: [10.21105/joss.00363](https://doi.org/10.21105/joss.00363). URL: <https://doi.org/10.21105/joss.00363>.
- Sommer, Philipp S. and Jed O. Kaplan (2017). "A globally calibrated scheme for generating daily meteorology from monthly statistics: Global-WGEN (GWGEN) v1.0". In: *Geosci. Model Dev.* 10.10, pp. 3771–3791. DOI: [10.5194/gmd-10-3771-2017](https://doi.org/10.5194/gmd-10-3771-2017).

B.0.2 Conference contributions

- Sommer, P. S., B. A. S. Davis, and M. Chevalier (2019a). "Github and Open Research Data; an example using the Eurasian Modern Pollen Database". In: *EGU General Assembly Conference Abstracts*. Vol. 21. EGU General Assembly Conference Abstracts, p. 5669. URL: <https://meetingorganizer.copernicus.org/EGU2019/EGU2019-5669.pdf>.
- Sommer, Philipp S., Basil A. S. Davis, Manuel Chevalier, Jian Ni, and John Tipton (2019b). "The HORNET project: applying 'big data' to reconstruct the climate of the Northern Hemisphere during the Holocene". In: *20th Congress of the International Union for Quaternary Research (INQUA)*. International Union for Quaternary Research. URL: <https://app.oxfordabstracts.com/events/574/program-app/submission/94623>.

- Sommer, P. S. (2018). "Psyplot: Interactive data analysis and visualization with Python". In: *EGU General Assembly Conference Abstracts*. Vol. 20. EGU General Assembly Conference Abstracts. Provided by the SAO/NASA Astrophysics Data System, p. 4701. URL: <http://adsabs.harvard.edu/abs/2018EGUGA..20.4701S>.
- Sommer, P. S., B. A. S. Davis, and M. Chevalier (2018a). "STRADITIZE: An open-source program for digitizing pollen diagrams and other types of stratigraphic data". In: *EGU General Assembly Conference Abstracts*. Vol. 20. EGU General Assembly Conference Abstracts. Provided by the SAO/NASA Astrophysics Data System, p. 4433. URL: <http://adsabs.harvard.edu/abs/2018EGUGA..20.4433S>.
- Sommer, Philipp S., Manuel Chevalier, and Basil A. S. Davis (2018b). "STRADITIZE: An open-source program for digitizing pollen diagrams and other types of stratigraphic data". In: *AFQUA - The African Quaternary*. Nairobi (Kenya): AFQUA. URL: <https://afquacongress.wixsite.com/afqua2018>.
- Sommer, P. and J. Kaplan (2017). "Quantitative Modeling of Human-Environment Interactions in Preindustrial Time". In: *PAGES OSM 2017, Abstract Book*, pp. 129–129.
- Sommer, P. (2016). "Psyplot: Visualizing rectangular and triangular Climate Model Data with Python". In: *EGU General Assembly Conference Abstracts*. Vol. 18. EGU General Assembly Conference Abstracts. Provided by the SAO/NASA Astrophysics Data System, p. 18185. URL: <http://adsabs.harvard.edu/abs/2016EGUGA..1818185S>.
- Sommer, P. and J. Kaplan (2016a). "Fundamental statistical relationships between monthly and daily meteorological variables: Temporal downscaling of weather based on a global observational dataset". In: *EGU General Assembly Conference Abstracts*. Vol. 18. EGU General Assembly Conference Abstracts. Provided by the SAO/NASA Astrophysics Data System, EPSC2016–18183. URL: <http://adsabs.harvard.edu/abs/2016EGUGA..1818183S>.
- (2016b). "Fundamental statistical relationships between monthly and daily meteorological variables: Temporal downscaling of weather based on a global observational dataset". In: *Workshop on Stochastic Weather Generators*. Vannes (France): University of Bretagne Sud. URL: <https://www.lebesgue.fr/content/sem2016-climate-program>.

Appendix C

New Software Tools - An Overview

This section mainly contains the latest version of the package, a short summary and an information table about where to find everything (Documentation, source code, etc.)

Need to write chapter C

C.1 Main packages

- psyplot
 - psy-simple
 - psy-maps
 - psy-reg
 - psyplot-gui
 - psy-strat
- straditize
- gwgen
- iucm
- EMPD
 - EMPD-admin
 - EMPD-viewer
 - EMPD-data
- POLNET
 - POLNET-viewer
 - POLNET-data

C.2 Other packages

- docrep
- sphinx-nbexamples
- model-organization
- funcargparse
- autodocsumm