Scientific Computing

Introduction

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Latest version available on Github, this PDF is version ebb6091.

Survey regarding preknowledge

or

menti.com

code <snip>

1. Who we are
2. What this course is about
3. How the class works
4. Prerequisites
5. How we grade
6. Resources
7. First assignment

Who we are

Johannes Schmidt <johannes.schmidt@boku.ac.at>

- Associate Prof. in Energy & Resource Economics at the Institute for Sustainable Economic Development
- Works on modeling of renewable energy systems in R, GAMS (and Python)
- Studied Computer Science at TU Wien

Who we are

Johannes Schmidt <johannes.schmidt@boku.ac.at>

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Peter Regner <peter.regner@boku.ac.at>

- PhD student at the Institute for Sustainable Economic Development
- Worked almost 7 years as Python developer in semiconductor industry
- Studied mathematics at TU Wien

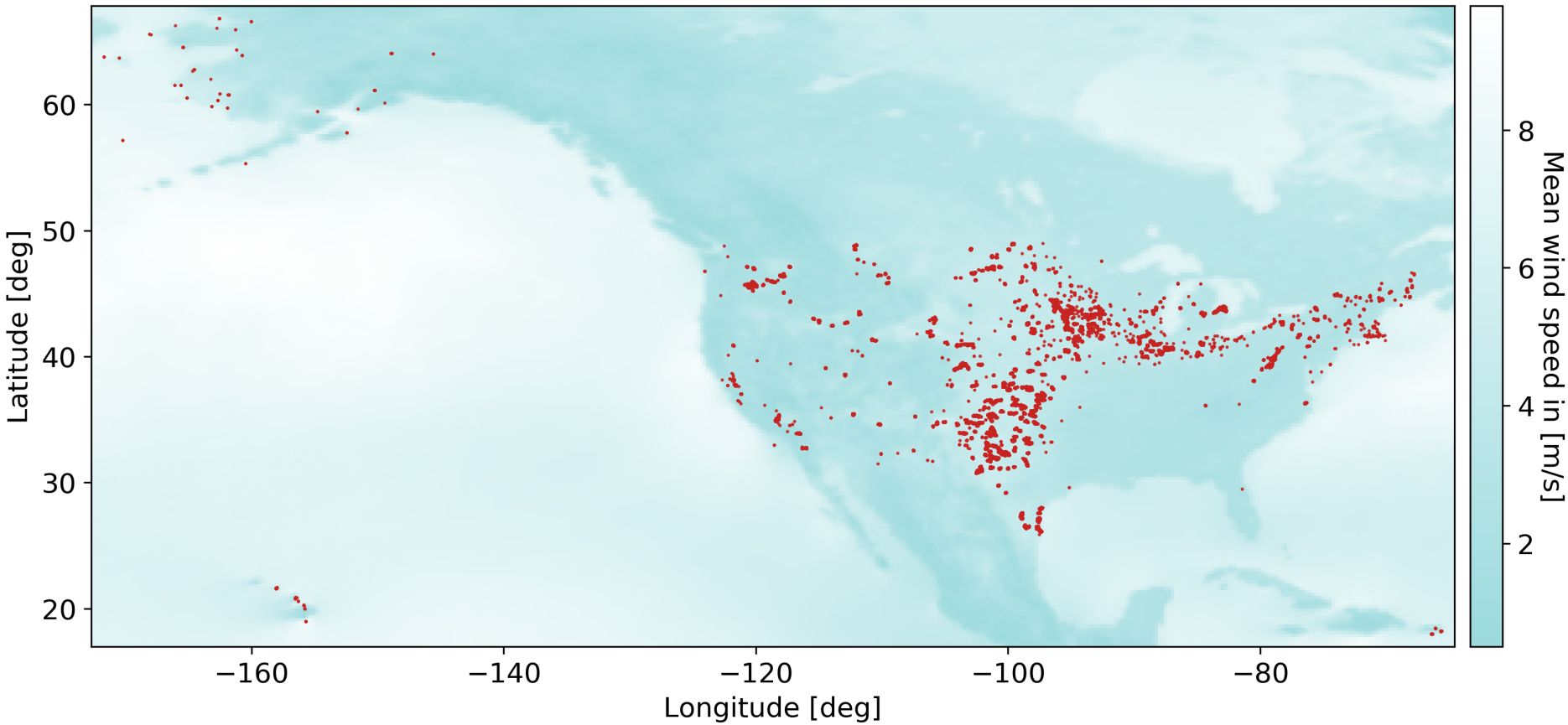
Aim of course

Learn to use programming as a tool in research

- Version control your code with Git and collaborate on Git(hub)
- Install Python, Python packages, and Jupyter notebook servers in Conda environments
- Start programming in python and understand flow features (loops and conditions) and functions
- Get an overview of the Python scientific ecosystem
- Use Python scientific stack packages (numpy, xarray)
- Use open (climate) data in your research projects
- Generate plots using matplotlib

Example use cases

Possible homework/application of presented know-how:
Mean wind speed and wind turbine locations in the US



How the class works

- 1.5 hours of lecture
- 1.5 hours of practical exercises
- Homework in groups

Dates

Date	Content
12.03.2020 13:00-16:15	Introduction
19.03.2020 13:00-16:15	Introduction to Git
26.03.2020 13:00-16:15	Installation of Python in Conda
02.04.2020 13:00-16:15	Start programming in Python
30.04.2020 13:00-16:15	Python scientific ecosystem
07.05.2020 13:00-16:15	Numpy and xarray, **Maybe skipped**
14.05.2020 13:00-16:15	Use open (climate) data
28.05.2020 13:00-16:15	Generate plots using matplotlib
04.06.2020 13:00-16:15	**Replacement date for 7th of May**

Prerequisites

- You should feel very comfortable with your respective operating system (Windows, Linux, Mac OS)
- Ideally, you have some experience with using a command line / terminal
- In a perfect world, you have programmed before

Grading scheme

- Organize in groups of 4 students
- Do homework together
- Be prepared to present homework individually ("Kreuzerlübung")

Resources

Slides, links and other material in this Github repository:
https://github.com/inwe-boku/lecture-scientific-computing

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Where/whom to ask questions?

- In a new Github issue, do not write emails to us:
  https://github.com/inwe-boku/lecture-scientific-computing/issues
- Your fellow peers in your group
- Ask us during class

First assignment (I)

Homework (due on 19th of March):

- register at github.com or any alternative GIT hoster (e.g. gitlab.com)
- install a GIT and gitk (see instructions (1) on next slide)
- click/browse quickly through links & tutorials (see on next slide)
- clone a repository, change a file and commit (see instructions (2) next slide)
- prepare one question about GIT and add it to the list: https://yourpart.eu/p/lecture-scientific-computing

First assignment (II)

(1) Install GIT & gitk

Installation on Linux:

on Debian based systems run the command:

```
sudo apt install git gitk
```

Installation on Windows:

1. install notepad++ (https://notepad-plus-plus.org/downloads/)
2. install git for windows (https://gitforwindows.org/). During the installation procedure, choose notepad++ as your preferred editor.

Configure name and mail address:

Run a terminal (windows: GIT bash) and run the command[1]:

```
git config --global user.name "My Name or Pseudonym"
git config --global user.email my-public-mailadress@example.com
```

[1] See also https://git-scm.com/book/en/v2/Getting-Started-First-Time-Git-Setup

First assignment (III)

(2) Clone the lecture repository and add a commit
Run a terminal (windows: GIT bash) and run the command:

```
git clone https://github.com/inwe-boku/lecture-scientific-computing
```

Then change a file of your choice and run:

```
git add <file-name-of-the-file-you-changed>
```

Explain your change in the commit message and close the editor.
Run gitk to check your commit.

First assignment (IV)

See also:
https://guides.github.com/introduction/git-handbook/
(especially the section "Example: Contribute to an existing repository")

More helpful resources about GIT can be found here:
https://github.com/inwe-boku/lecture-scientific-computing/blob/master/lecture01-git-version-control/links.rst

First assignment (V)

Warning: you will need to push your homework to a public Github repository. Your Github account is your business card for programmers – your homework will be part of it. You can create a separate Github account only for this course to be anonymous or your group deletes the repository after the semester, if you don't want your homework to remain public. Note: the name and mail address chosen during the GIT installation will be public too.