Scientific Computing

Introduction

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Latest version available on Github, this PDF is version a9adcab.

Survey regarding preknowledge

menti.com

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

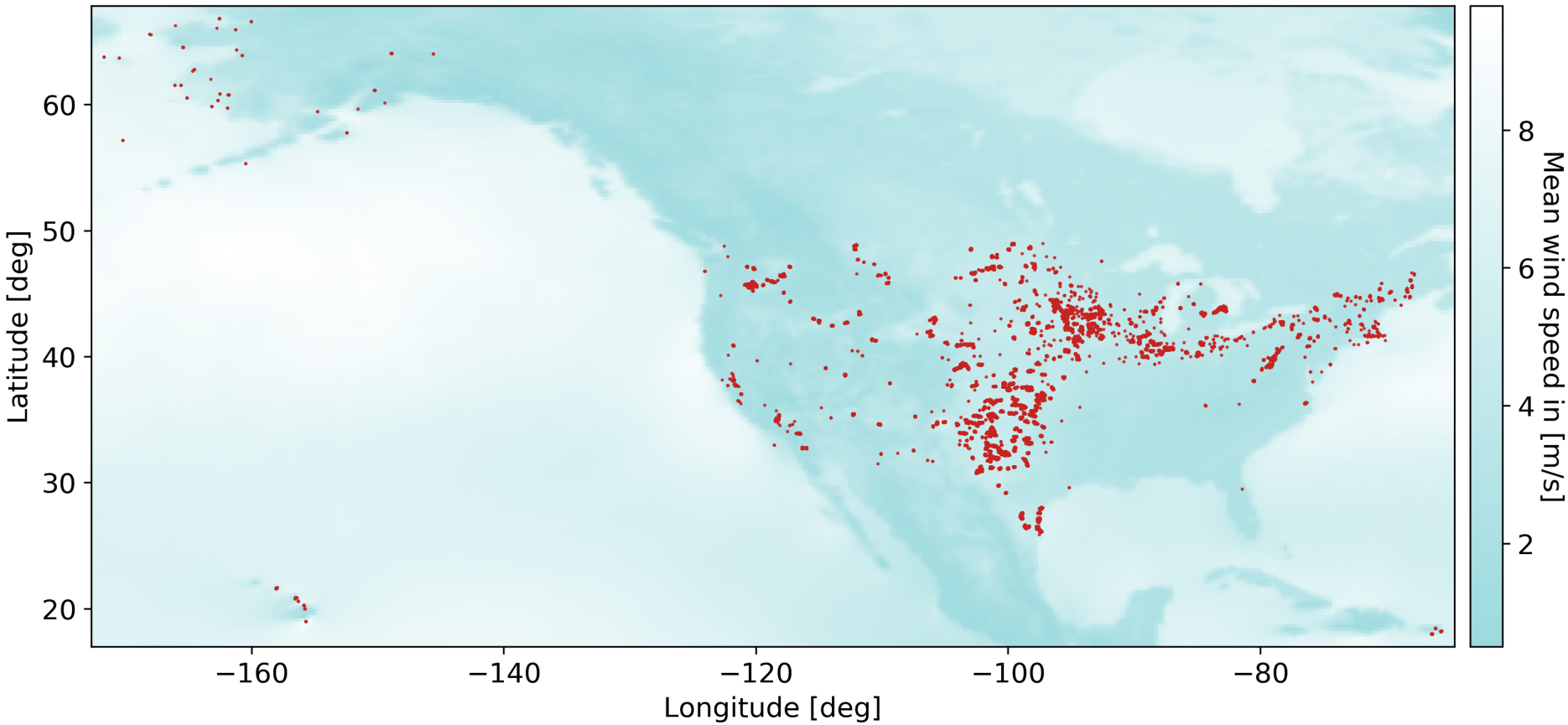
Aim of course

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 edit any arbitrary file, e.g. add "I was here" to REDAME.md and run:

```
cd lecture-scientific-computing
git add path/to/file-you-changed
git commit -m 'I changed a file'
```

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.