# Scientific Computing

Introduction

Peter Regner, Johannes Schmidt

Institute for Sustainable Economic Development, BOKU, Wien

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# 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

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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

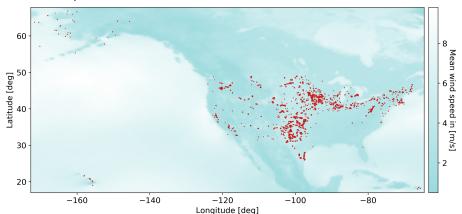
### Aim of course

### 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, <b>Maybe skipped</b>
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<sup>1</sup>:

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

<sup>&</sup>lt;sup>1</sup>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>
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.