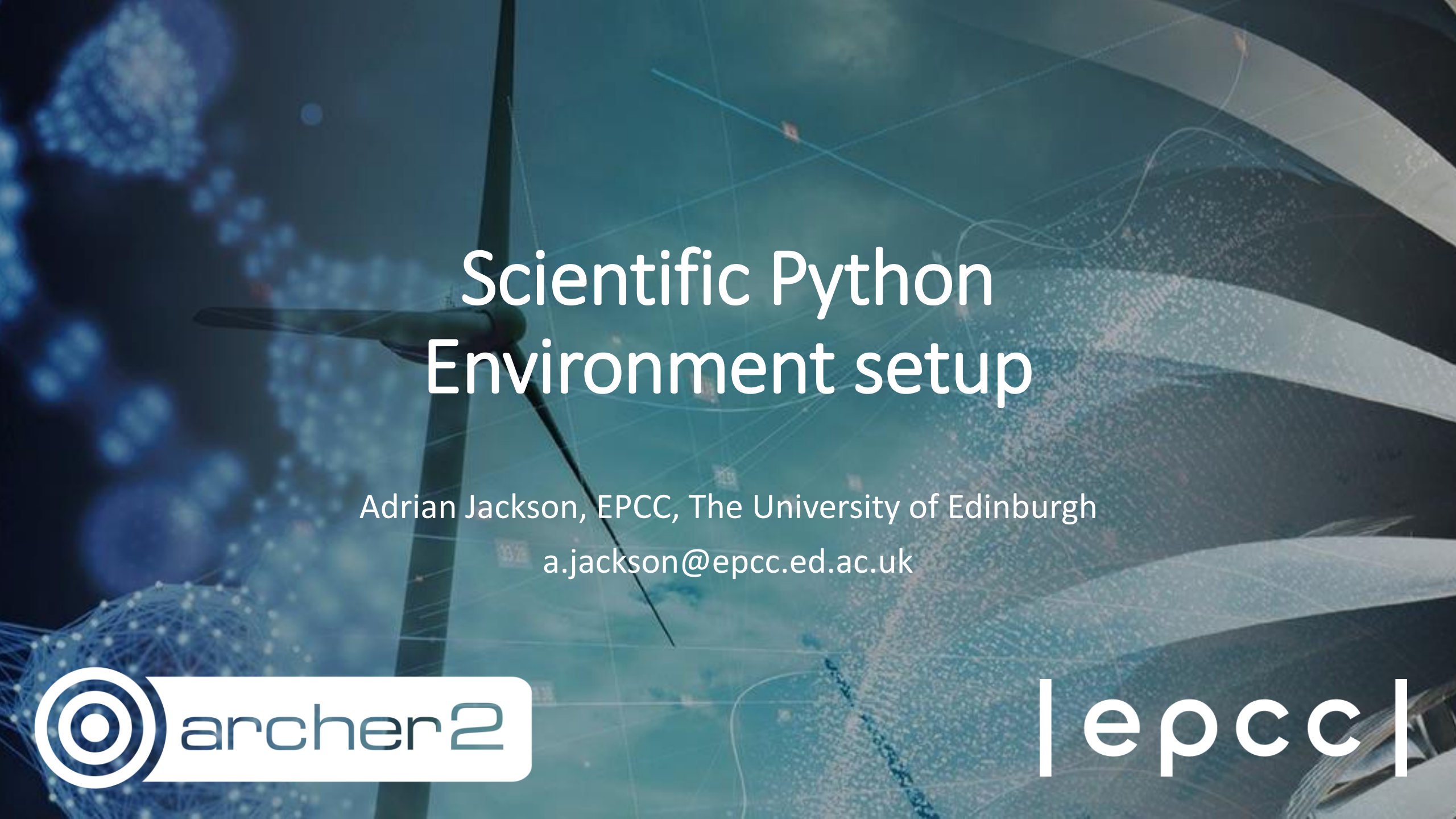

# Scientific Python Environment setup

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archer2

epcc

# Reusing this material

# Partners

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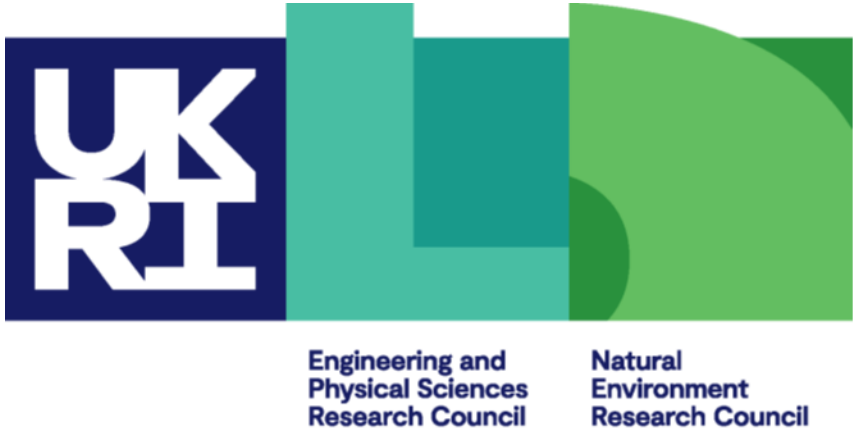


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# Using Python and Jupyter

- You can install Python/Jupyter on your own laptop
  - Easiest way is to use anaconda:
    - https://www.anaconda.com/download/
  - This will contain most of what we require for the course
- It is also possible to use Python and Jupyter on ARCHER2
- If you want to do this on ARCHER2, you can do the following once logged in:
  - `module load cray-python`
  - `export PYTHONUSERBASE=/work/t01/t01/auser/.local`
    - You will need to change t01 to the project code for your project, and auser to your username
  - `export PATH=$PYTHONUSERBASE/bin:$PATH`
  - `# source <<path to virtual environment>>/bin/activate  # If using a virtualenvironment uncomment this line and remove the --user flag from the next`
  - `pip install --user jupyterlab`

# Connecting to Jupyter on ARCHER2

- Start the Jupyter server on the login node:
  - `export JUPYTER_RUNTIME_DIR=$(pwd)`
  - `jupyter lab --ip=0.0.0.0 --no-browser`
- This will produce something output like this:

```
[I 2022-02-16 16:11:22.096 ServerApp] Serving notebooks from local directory: /home2/home/z19/z19/adrianj
[I 2022-02-16 16:11:22.096 ServerApp] Jupyter Server 1.13.5 is running at:
[I 2022-02-16 16:11:22.096 ServerApp] http://ln04:8888/lab?token=2b71da8e6435331419l4f0475081d73e113a630e2ffdc727
[I 2022-02-16 16:11:22.096 ServerApp]  or http://127.0.0.1:8888/lab?token=2b71da8e6435331419l4f0475081d73e113a630e2ffdc727
[I 2022-02-16 16:11:22.096 ServerApp] Use Control-C to stop this server and shut down all kernels (twice to skip confirmation).
[C 2022-02-16 16:11:22.134 ServerApp]

    To access the server, open this file in a browser:
        file:///home2/home/z19/z19/adrianj/.local/share/jupyter/runtime/jpserver-5600-open.html
    Or copy and paste one of these URLs:
        http://ln04:8888/lab?token=2b71da8e6435331419l4f0475081d73e113a630e2ffdc727
     or http://127.0.0.1:8888/lab?token=2b71da8e6435331419l4f0475081d73e113a630e2ffdc727
```

- To connect to the Jupyter server from your local browser you need to forward the specific port using SSH:
  - `ssh <username>@login.archer2.ac.uk -L<port_number>:localhost:<port_number>`
  - You need to ensure that your SSH to the same login nodes as your server is running on
  - Then paste the `http://127.0.0.1...` URL that was printed out when you started up Jupyter in your local browser and it should connect

# Introduction

- Start the `lectures/dev-intro/intro.ipynb` in your Jupyter notebook/lab


- You can read the notebook here instead and use the python interpreter to do the exercises:
  - https://github.com/EPCCed/archer2-python/blob/master/lectures/dev-intro/intro.ipynb