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# Scientific Computing Skills

At Aalto University, in Finland, in the Nordics,  
...and beyond

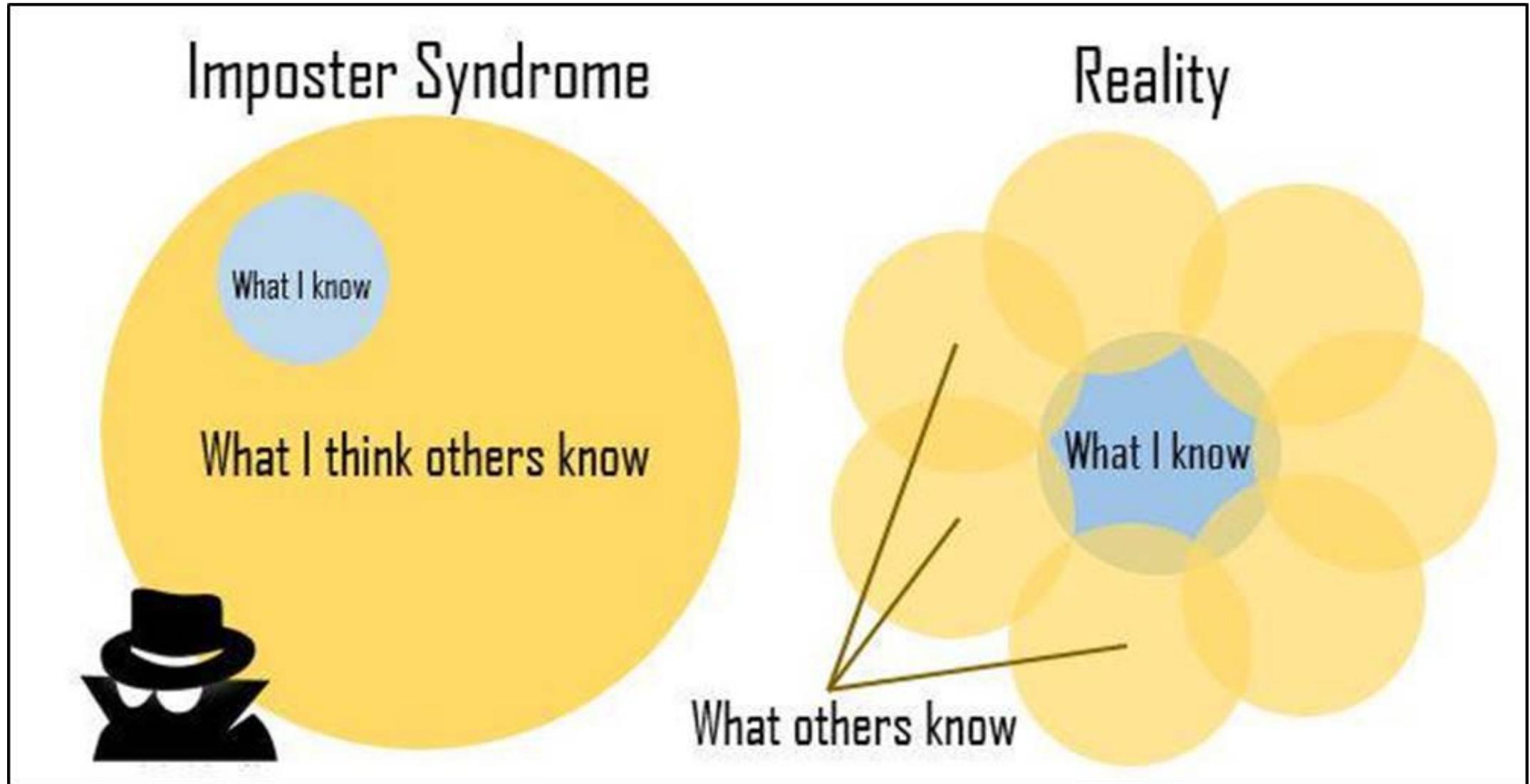
Enrico Glerean

# Briefly about myself

## Enrico Glerean, DSc.

- **Staff scientist and data agent** (background in neuroimaging), training and supporting researchers with handling personal data (anonymization, secure computing), medical images, clinical trials, research ethics and research integrity (AI and new technologies), statistics, open science.
- Other affiliations/COI: **CodeRefinery** (Nordic network to teach computational reproducibility), **Finnish Reproducibility Network** (National network to raise awareness in reproducibility), Support Pool of Experts at the **European Data Protection Board** (open training materials on personal data, AI, and cybersecurity), **Data Steward training program for Tampere University**

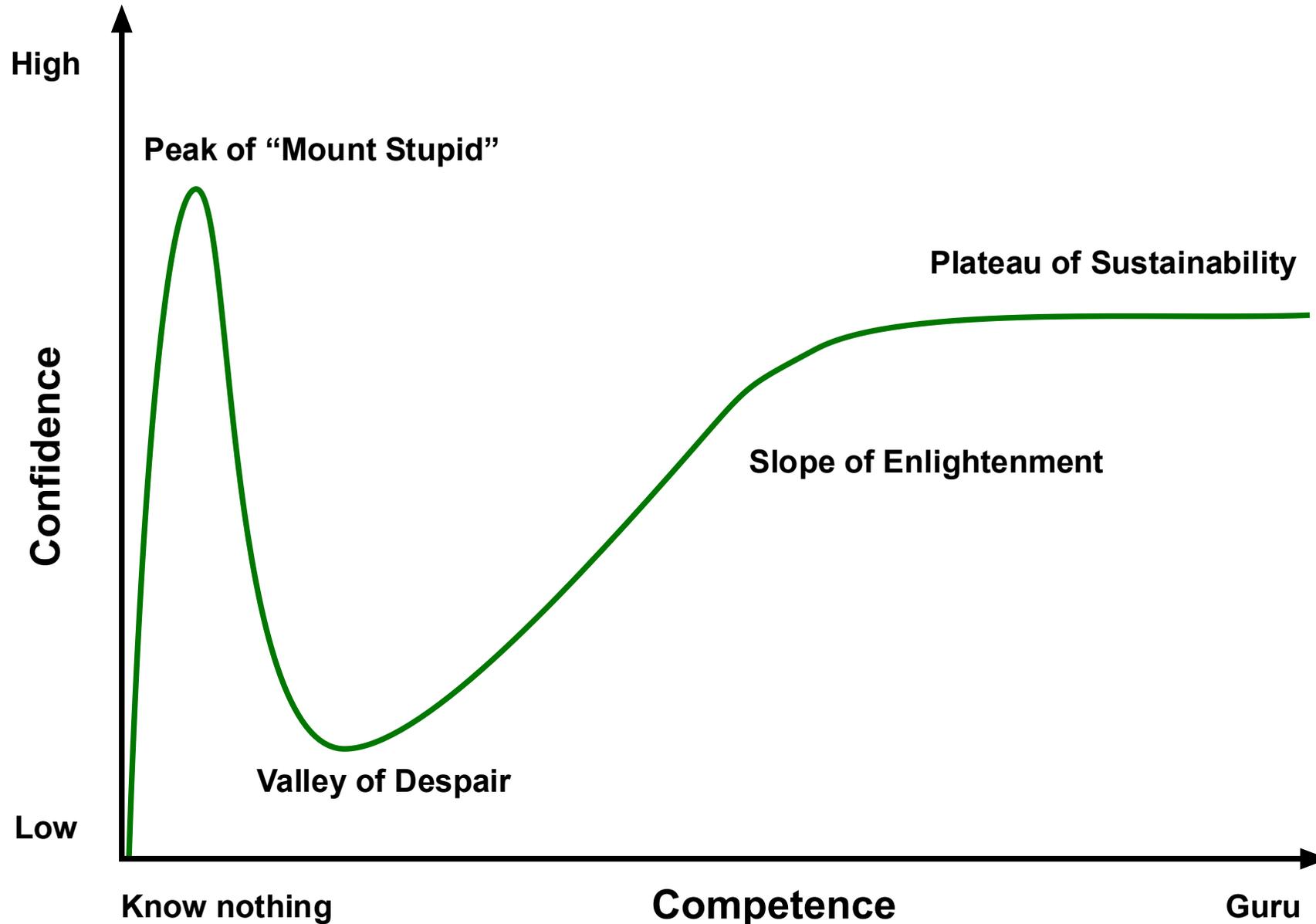
# A reminder: imposter syndrome



**A!**

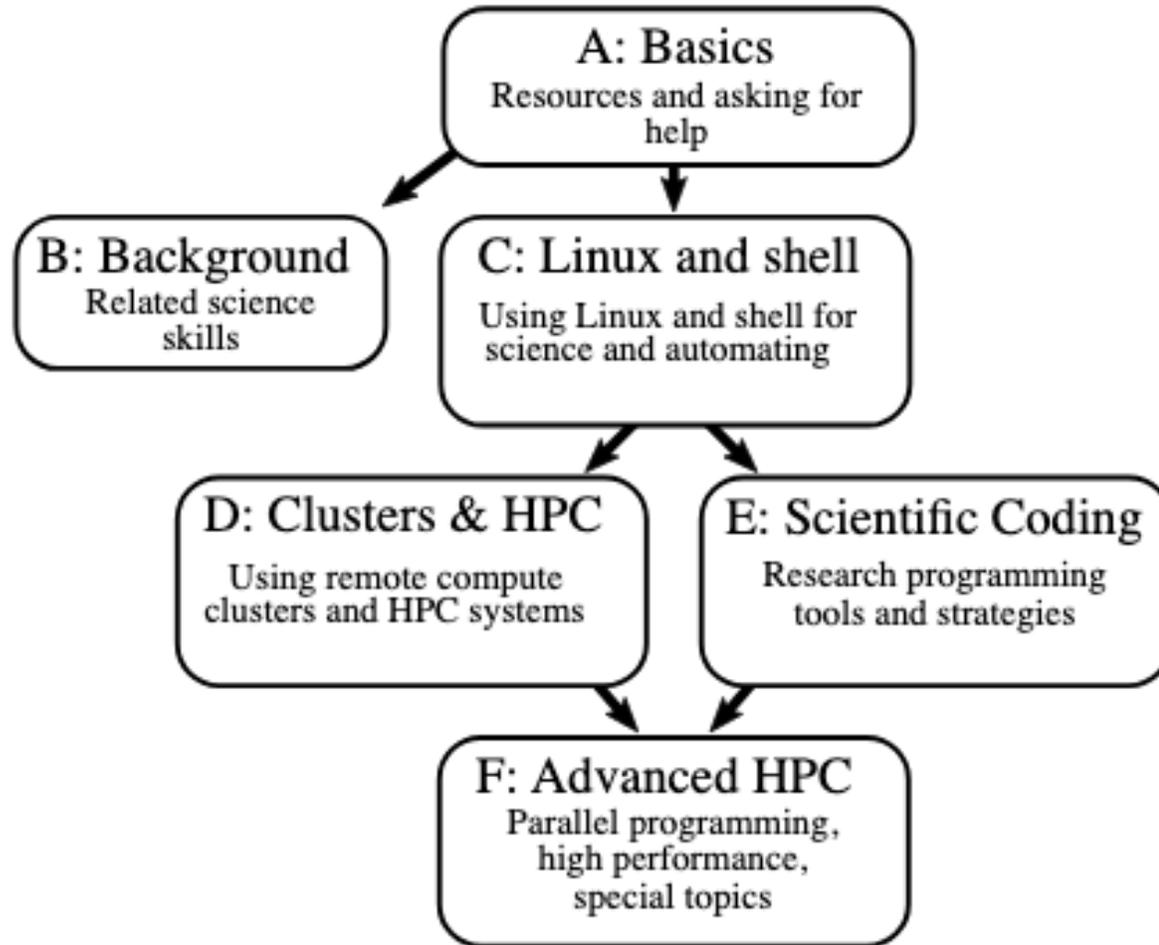
Image by David Whittaker (@rundavidrun) Used with permission

# Dunning–Kruger Effect

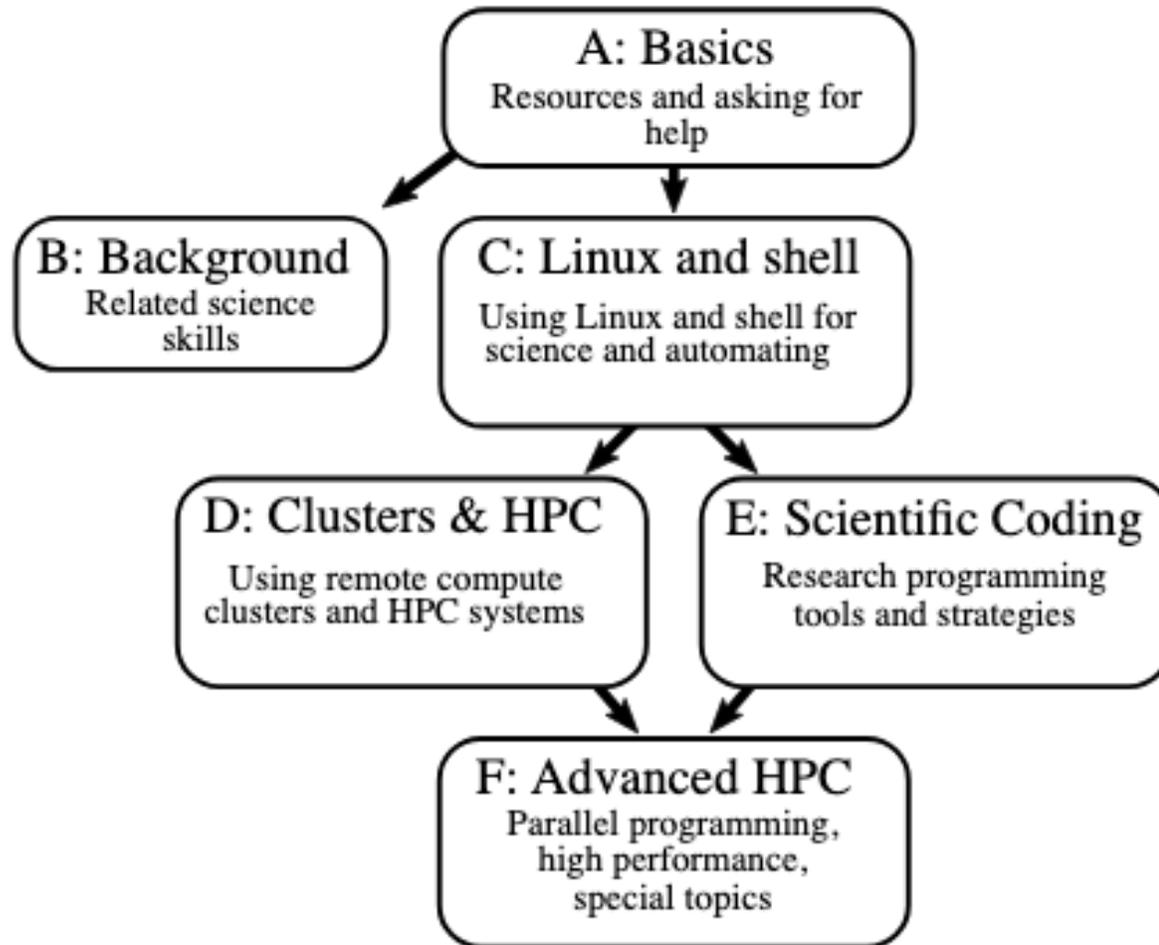


The **Dunning–Kruger effect** is a cognitive bias that describes the systematic tendency of people with low ability in a specific area to give overly positive assessments of this ability. (Wikipedia)

# Scientific Computing Skills



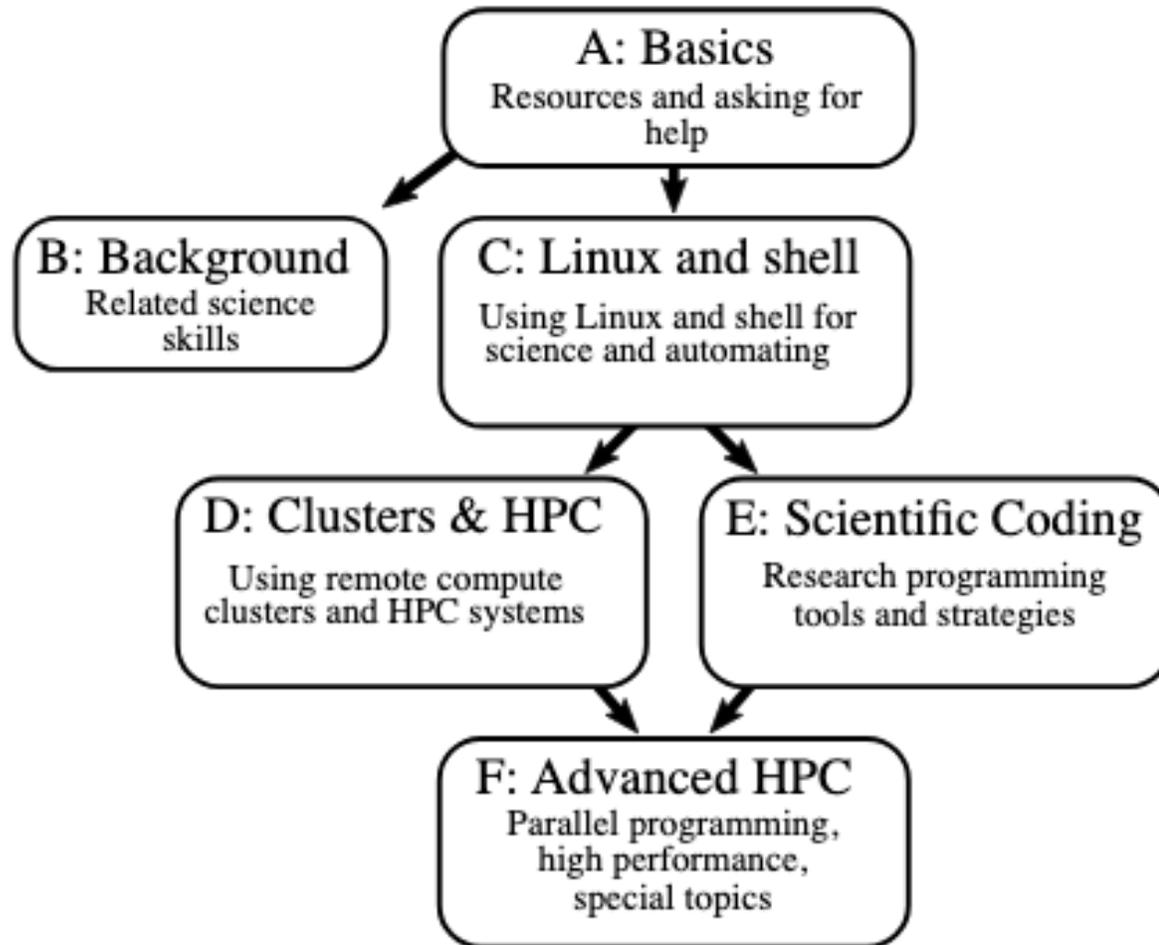
# Scientific Computing Skills



## A. Basics

- Understand what scientific computing is and what resources exist.
- Learn a sensible **research workflow** and **where to get help**.
- **Set up your own computer** for scientific work.
- **Install** the core tools you will need on Linux, macOS, or Windows.

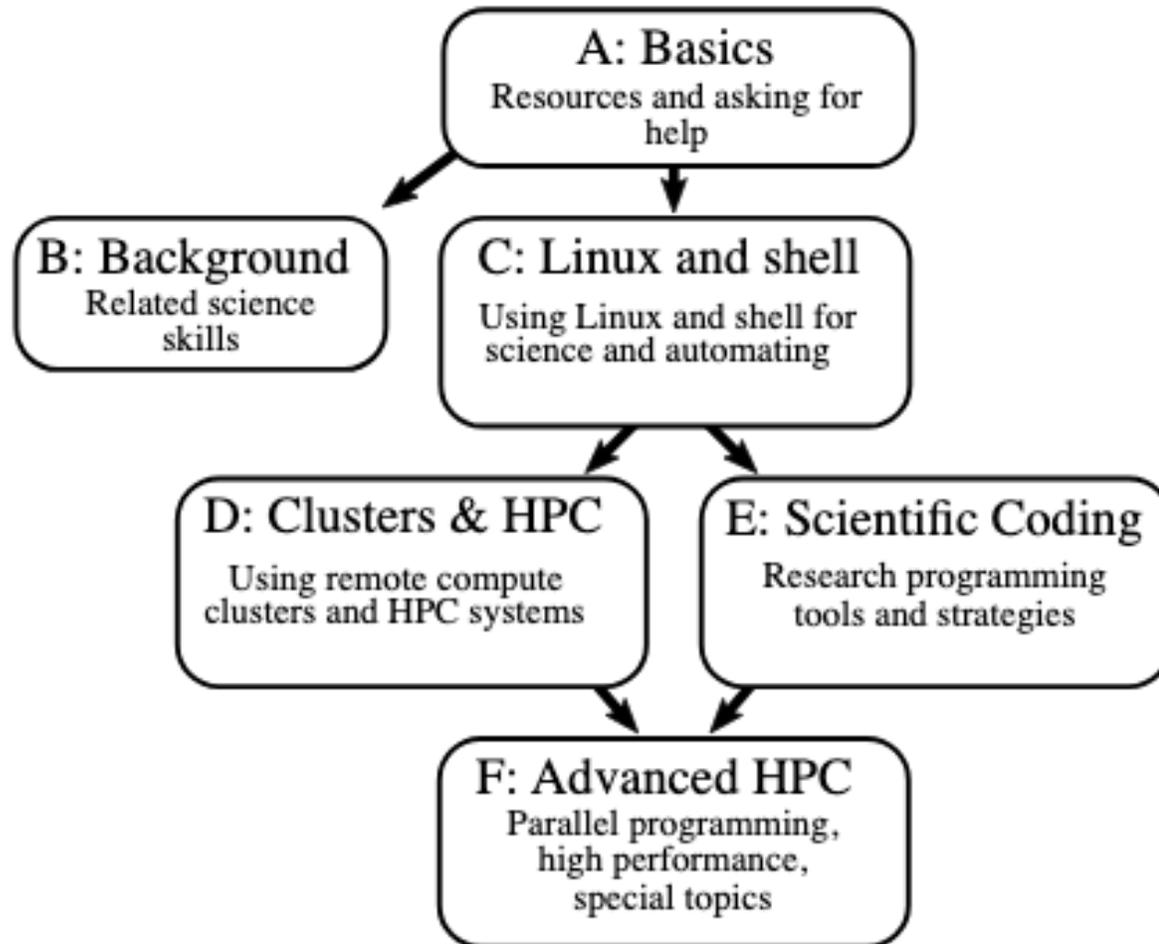
# Scientific Computing Skills



## B. Related science skills

- **Organize research data** so it stays usable and well structured.
- Use **Jupyter** notebooks when self-documenting analysis is helpful.
- Create clear, **publication-quality figures**.
- Write papers and reports in **LaTeX**.
- Design concise scientific **posters**.

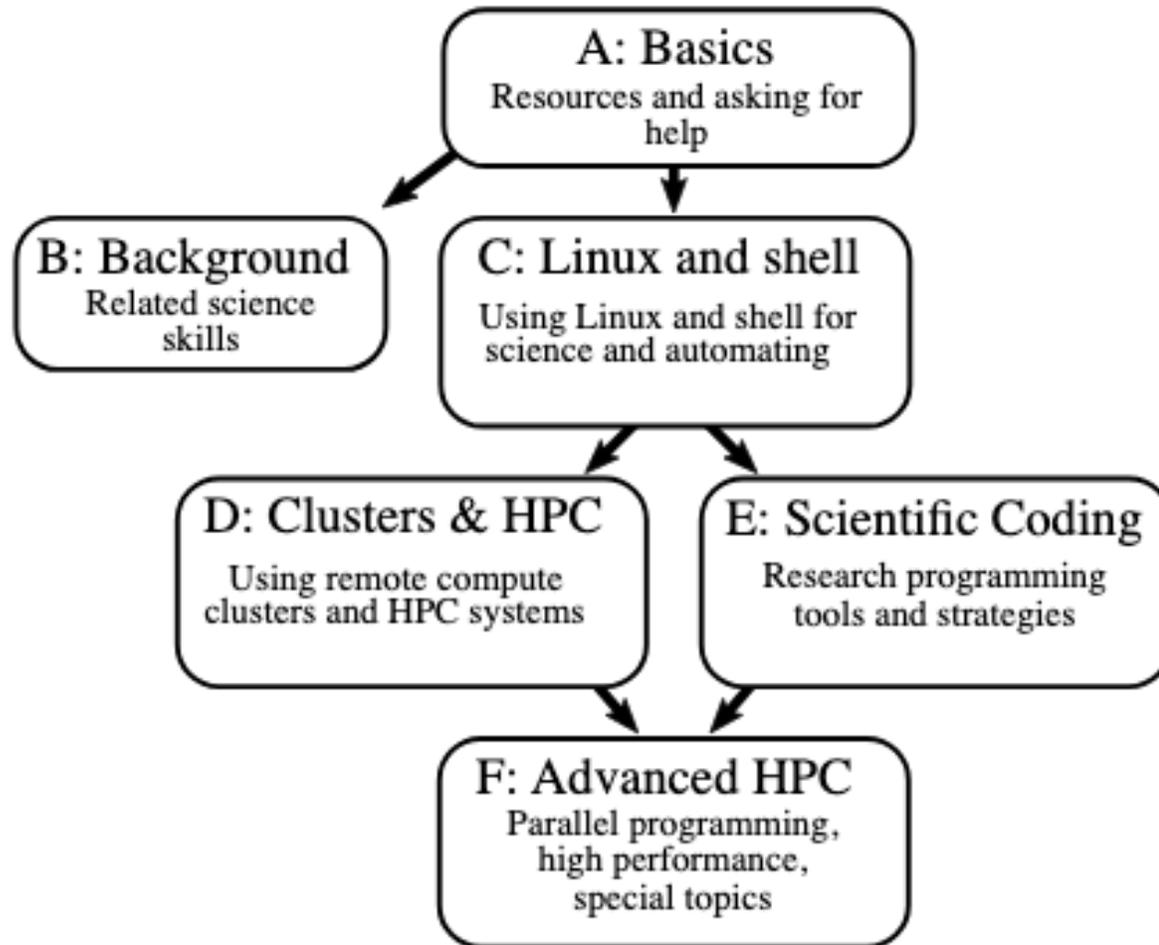
# Scientific Computing Skills



## C. Linux and shell

- Work comfortably in the **shell/command line**.
- Use a text editor or IDE effectively.
- **Automate repetitive tasks** with shell scripts.
- Use **Git** for tracking changes and collaboration.
- Connect to remote systems with **SSH**.
- Use **Make/SnakeMake** to automate multi-step workflows

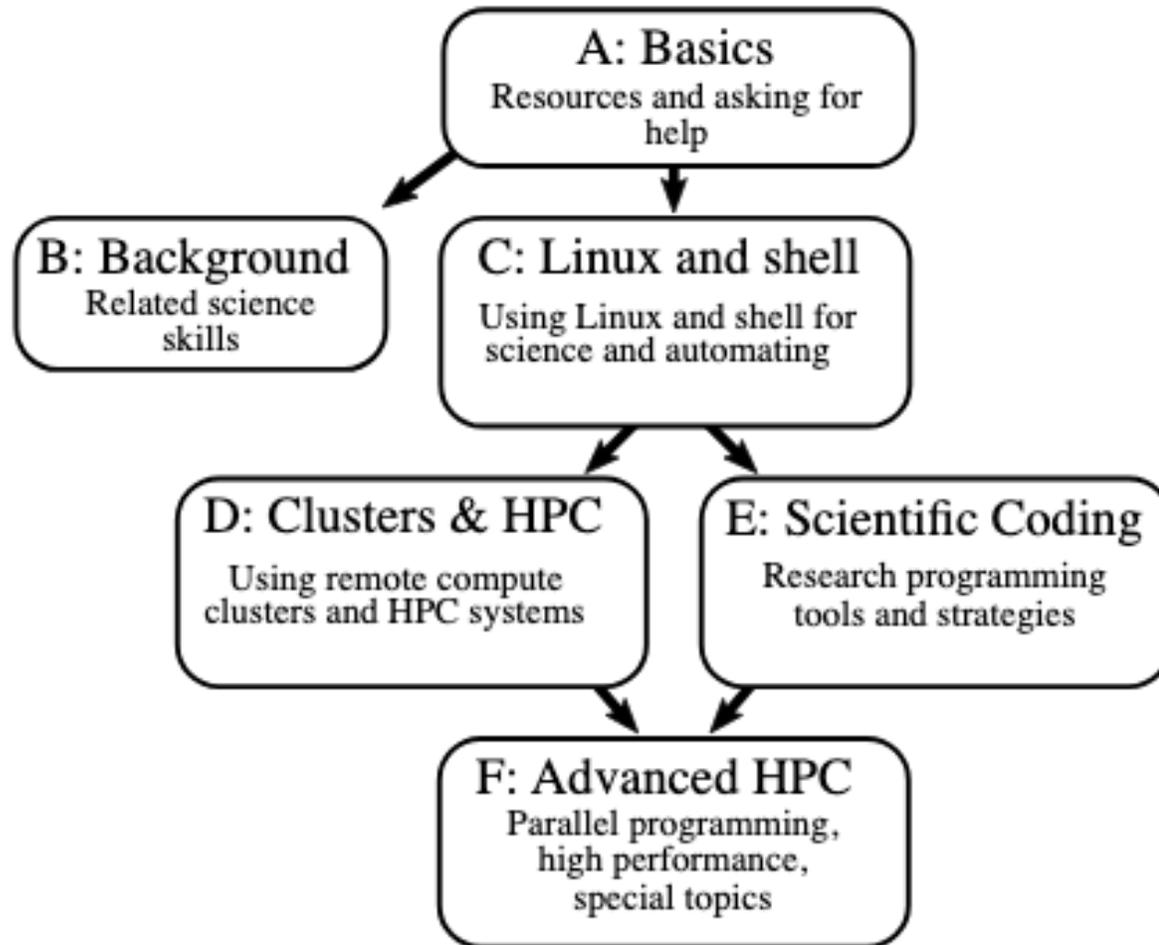
# Scientific Computing Skills



## D. Clusters and high-performance computing

- Understand what **HPC** is and when to move beyond your own computer.
- Use environment **modules** to find and load software on clusters.
- Submit, monitor, and manage jobs with a batch system such as **Slurm**.
- Handle HPC **storage** correctly and avoid I/O bottlenecks.
- Run **parallel jobs** and recognize common parallel models.
- Automate larger **cluster workflows** with more advanced shell usage

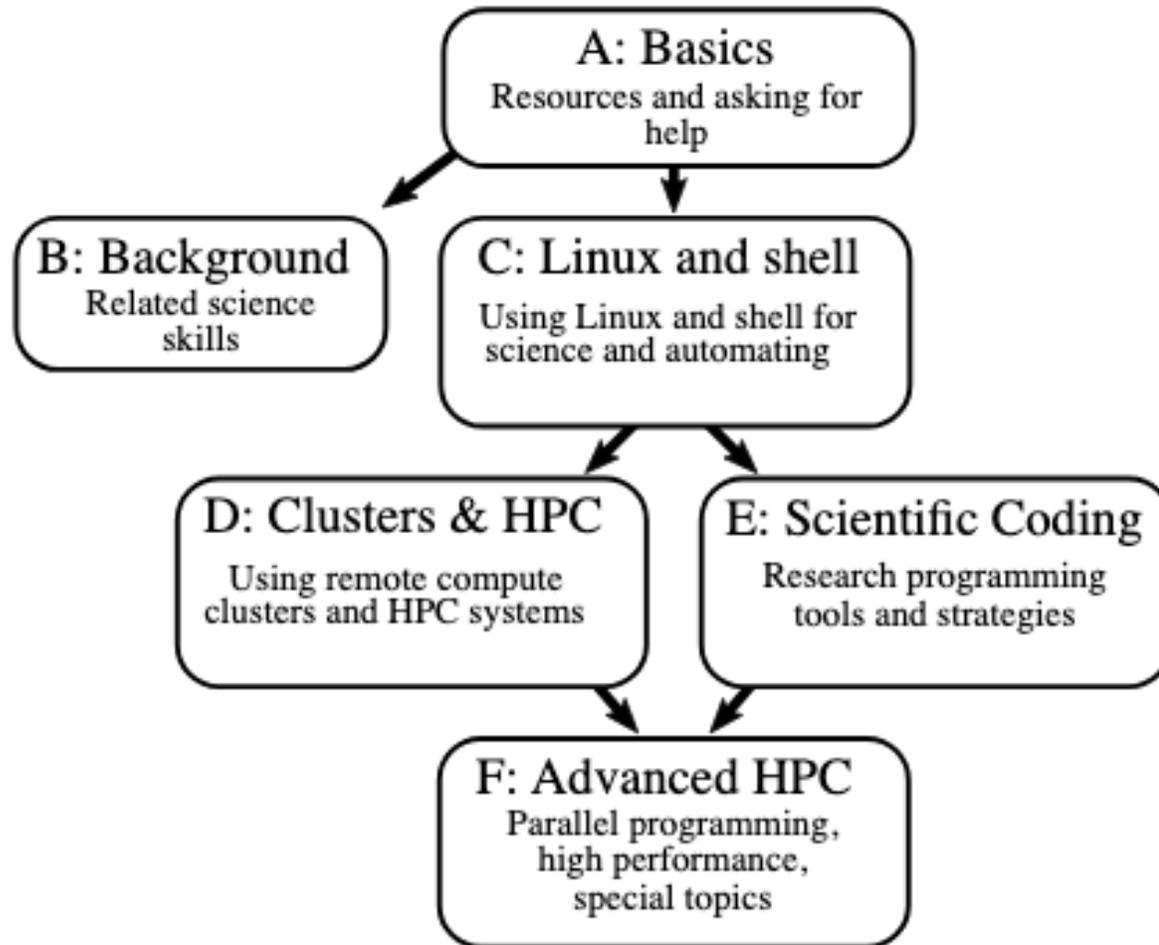
# Scientific Computing Skills



## E. Scientific coding

- Structure **code** into clean, **modular** components.
- Write **tests** so software stays reliable.
- **Profile** code to find performance bottlenecks.
- **Debug** systematically.
- Understand **software licensing** and **sharing**.
- **Document** code so others can use and contribute to it.
- Make research workflows more **reproducible**.

# Scientific Computing Skills



## F. Advanced high-performance computing

- Learn **parallel programming** models in depth.
- **Program GPUs** for high-performance workloads.
- Learn **MPI** well enough to build distributed-memory applications.

**We are all at different points in our life-long learning path.**

**So who can help you?**



**CODE REFINERY**



**A?**

**RDM  
& Open Science  
Training**



**A!**

**Introduction to Scientific Computing and HPC**

**Hands-on Data Protection**

**How to Debug Code**

**Software Design for Scientific Computing**

**Python for Scientific Computing**

**Introduction to Julia**

**Introduction to MPI**

**Linux Shell Basics**

**Linux Shell Scripting**

**Matlab Basics**

**Matlab Advanced**

**Git version control (CodeRefinery)**

**Reproducibility (CodeRefinery)**

**Containers for High Performance Computing**

**Parallelization**

**Responsible use of Generative AI in assisted coding**

# CSC training calendar

2026

April

Onsite

**CSC Spring School on Computational Chemistry 2026**

8. - 10.4.2026

Bioinformatics and Life Sciences

Chemistry

High Performance Computing

Beginner

Intermediate

Online

**Microbial community / environmental DNA analysis with Chipster**

14. - 15.4.2026

Bioinformatics and Life Sciences

Beginner

Hybrid

**Practical Deep Learning**

14. - 15.4.2026

AI and Data Analytics

LUMI

Intermediate

Hybrid

**Moving your HPC workloads to LUMI**

22. - 23.4.2026

LUMI

Beginner

May

Hybrid

**Nordic Data Stewardship Network's Hybrid Seminar**

6.5.2026

Data Management

Beginner

**Introduction to GPU Programming**

11. - 13.5.2026

High Performance Computing

Programming

Onsite

**LUMI Profiling and Optimization Workshop**

11. - 13.5.2026

Cloud Computing

High Performance Computing

LUMI

Advanced

Hybrid

**Data Analysis with R**

12. - 13.5.2026

AI and Data Analytics

Beginner



<https://csc.fi/en/trainings/training-calendar/>

# Aalto Open Science Network trainings (open to the world)

<https://www.aalto.fi/en/services/training-in-research-data-management-and-open-science>

<https://www.youtube.com/@aaltoresearchservices>



**Demystifying research software publishing, Mar 12,...**

Learn about research software publishing with Luca Ferranti and the RSEs.  
12.3.2026 13:00–14:30 (UTC +2) | Ev...



**Introduction to Research Data Management, Mar 1...**

Get to know the basics of RDM.  
17.3.2026 13:00–14:30 (UTC +2) | Ev...



**Data storage and management for Aalto...**

Learn best practices in data storage at Aalto University.  
26.3.2026 13:00–14:30 (UTC +2) | E...



**Qualitative methods and research ethics review, Apr 14, 2026**

Learn about ethical review at Aalto University.  
14.4.2026 13:00–14:30 (UTC +3) | E...



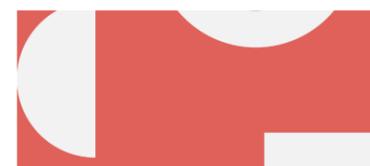
**REDCap survey tool for Aalto researchers, Apr 21...**

Learn about using REDCap at Aalto University.  
21.4.2026 13:00–14:30 (UTC +3) | Ev...



**Personal data in research, Apr 23, 2026**

Learn about handling personal data.  
23.4.2026 13:00–14:30 (UTC +3) | E...



**AI in research work - workshop, Apr 28, 2026**

Learn about using artificial intelligence (AI) tools in research.  
28.4.2026 9:30–15:30 (UTC +3) | Ev...



**Responsible and ethical use of laboratory...**

Learn about responsible and ethical use of laboratory resources.  
5.5.2026 13:00–14:30 (UTC +3) | Ev...



**Workshop on anonymising research data...**

Learn about anonymising research data.  
7.5.2026 13:00–14:30 (UTC +3) | Eve...

# LUMI AI Factory trainings

<https://lumi-ai-factory.eu/trainings/>

## OUR UPCOMING TRAINING SESSIONS



### LUMI related training opportunities

Date  
13.11.2025–3.12.2027

Location  
Online / Hybrid / On-site

[Learn more](#)



### Practical Deep Learning

Date  
14.4.2026–15.4.2026

Location  
Espoo, Finland

[Learn more](#)



### Moving your AI training jobs to LUMI: A hands-on workshop

Date  
11.6.2026–12.6.2026

Location  
Tromsø, Norway

[Learn more](#)



**And you can get ECTS!**

# SCI-L1010 in Sisu and MyCourses!

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☰

🏠 Main course page

▼ Course homepage

Announcements

Frequently Asked Questions

Requesting evaluation and credits

▼ Modules 2025/26

▼ Module 1

SCS1: 9/Sep-22/Oct  
CodeRefinery Fall 2025

SCS7: 17-26/March  
CodeRefinery Spring 2026

▼ Module 2

SCS2: 25-27/Nov/2025  
Python for Scientific Computing

▼ Module 3

SCS3: Jan/2026 Introduction to Scientific Computing and HPC

## SCI-L1010 - Scientific Computing Skills, Lectures, 1.8.2025-5.6.2026

Syllabus

Course Course feedback

### Course homepage

## Welcome to Scientific Computing Skills 2025-2026!

This is an umbrella course for multiple hands-on trainings provided by **Aalto Scientific Computing** and/or by partner organisations such as **CodeRefinery** and **CSC IT Center for Science**.

### → Enroll via SISU!

Today, computing skills are essential not only in academic research but also across industries. Whether you plan to be a coder or a non-coder collaborating with software developers, understanding the tools and speaking the same technical language will make you more effective. **This course focuses on computational tools for academic research and reproducibility:** ensuring you can conduct computational research efficiently, transparently, and to the highest standards. It follows a “**pick your own adventure**” approach: we are all diverse and come from different backgrounds. When you join a new research group the tools they use may be new to you: it could be Git, the Linux shell, a specific programming language,... you name it! **This course helps you bridge those technical gaps.** By selecting the modules most relevant to your work, you can earn up to 5 ECTS credits within one academic year.

Please note that **all modules are also open to any researcher** who wants to strengthen their skills without needing credits; we use this MyCourses space to submit homework and track completed modules for those who need credits. **We will add more trainings throughout the year when more events are announced. Come back to this page for updates.**

A!

**And remember, the good enough practices are often better  
than the best practices**

# Continuum of practices in (data) science

I do not want  
to do this job  
anymore

Bare minimum  
practices

Good enough  
practices

Best practices in  
data & project  
management



A single folder for all projects where everyone can write  
No backup strategy  
No README files  
No comments on code  
No version control  
No separation between raw/derivative data  
No meaningful filenames  
No history log  
No way to replicate past analysis  
No way for external person to know what's going on

(Open) data archived with DOI  
Data versioning with git-annex/DVC  
Registered protocols for data collection  
GIT version control + branches & tags  
(Open) code on GitHub + archived w DOI  
Unit tests and continuous integration  
Singularity/Apptainer/Docker container  
Automation with Make/Snakemake  
Consistent folder structure across projects  
Extensive documentation  
Collaboration tools (Zulip, Slack, GitHub, etc)

**A!**

<https://scicomp.aalto.fi/scicomp/rcr-scicomp/>

<https://vastuullinentiede.fi/en>