Scientific computing
- computing as a tool for doing science

Computer science
- the study of computation
“A mathematician is a device for turning coffee into theorems” – Erdős / Rényi

requirements ➔ code

thought process

data ➔ code

insight ➔ code
SCIENTIFIC COMPUTING

Try out an idea ✪ see what happens ✪ refine your idea ✪ try something else ✪ iterate ... ✪ share what you’ve learnt
CODE AT THE SPEED OF THOUGHT

- Concise one- or two-liners for one-off tasks
- Rich, expressive libraries & glue code
Scientific computing

= Python + numpy + plotting + pandas + Jupyter notebooks

First I ran this cell up here

And now this cell is producing strange answers

Then this one, I think.
Lecture notes from IA OOP

2. Use a build tool

Build tools facilitate a wide variety of build automation tasks:
- **Compiling**: Compiling source code into machine code
- **Dependency management**: Identifying and downloading third party libraries
- **Automated tests**: Executing tests and reporting failure
- **Packaging**: Prepare artifacts for deployment

Goal is to make life simpler with a repeatable and automatable build configuration.

**Maven** is the most widely adopted built tool in the Java ecosystem.

Modularity and Code reuse

- You've long been taught to break down complex problems into more tractable sub-problems.
- Each class represents a sub-unit of code that (if written well) can be developed, tested and updated independently from the rest of the code.
- Indeed, two classes that achieve the same thing (but perhaps do it in different ways) can be swapped in the code.
- Properly developed classes can be used in other programs without modification.
- Java also has the notion of **packages** to group together classes that are conceptually linked.

How do we maximise the chance our classes are reused?

Bad advice for scientific computing
Look at each line of your code and ask yourself: ‘does this spark joy?’ If not, delete it.
while working

- imports
- experiment 1
- debug code
- tweaked experiment 1
- experiment 2
- update to experiment 1
- forgotten import

after you’ve finished

- imports
- utility functions
- run-once setup code
- functions that implement your solutions
- submit solutions to autograder
0. Programming in Python
language quirks

1. Numerical computation
   numpy
2. Plotting data
   matplotlib

3. Working with data
   pandas
   A. Data scraping recipes

ASSESSMENT
(maths paper mark = 92% exam + 8% Scientific Computing ticks)

No written exam

Four ticks, each marked pass/fail
Ticks 1 and 2: pass the autograder & submit notebook by 22 Jan
Ticks 3 and 4: submit pdfs and notebook by 29 Jan

Some of you will have a viva.
Impact of redistribution on inequality and mobility

GOALS. This report analyses the relationship between inequality and social mobility, as it is affected by taxation and redistribution.

METHODOLOGY. I investigated on a system of economic exchange of a flat-rate tax on wealth combined with a universal basic income. For each tax rate in a range of values, I simulate a population of 10,000 individuals, and measured the GINI coefficient. I ensure my simulator has reached steady state by magic.

RESULTS:

CONCLUSION: There is no tradeoff between inequality and mobility: redistribution not only reduces inequality, it also increases mobility.
The autograder will run wherever you run Python3
MY CODE PASSED TEST 2. BUT IT WAS BUGGY CODE, AND IT TOOK ME AGES TO DEBUG AND PASS TEST 3.

YOUR GRADER SUCKS.

Scientific computing isn’t about meeting requirements, it’s about discovery.

- chart your own path
- write your own tests
- invent a few small test cases
- work them out with pen and paper
- make sure your code agrees
Can I use ChatGPT?

HM, HOW DO SCIENTIFIC COMPUTING PROBLEM?

HM, HOW DO I E SIC! COMUTING PROBLEM?

HM, HOW DO SOLVE THIS ENTIRE SCIENTIFIC COMPUTING PROBLEM?

WOW, AI IS LIKE A TUTOR!!

WOW, - ChatGPT

- ChatGPT

- ChatGPT

- ChatGPT

THIS = HOMEWORK LIKE A TUTOR!!
Can I use ChatGPT?
Yes, feel free.

Can I use ChatGPT to save me time and effort?
Unlikely.

Can I use ChatGPT to sharpen my thinking?
Yes !!! 👍🔥👍🔥👍🔥👍
Help and support

- Moodle help forum
- Helpdesk sessions early in Lent term
- Optional hints-and-tips lecture early in Lent term