Welcome!

Artificial Intelligence/Machine Learning Bootcamp

August 5-16, 2024

@BrookhavenLab

Agenda

- Welcome (logistics and expectations)
- Overview of DOE and BNL
- Introduce OEP
- Introduce CSI
- Motivation for Bootcamp
- Intro to Python

This Week's Schedule at a Glance

Intro to Python Modules (Monday through Wednesday)

- Introducing Scientific Computing
- Python Fundamentals
- Graphing
- Functions and Logic
- Probability and Statistics
- Random Numbers and Algorithms
- Capstone Project – Make a Game!

This Week's Schedule at a Glance (cont.)

Thursday

- **Internship Day!** *Meet current interns and learn about their experiences in the SULI and CCI programs at BNL*

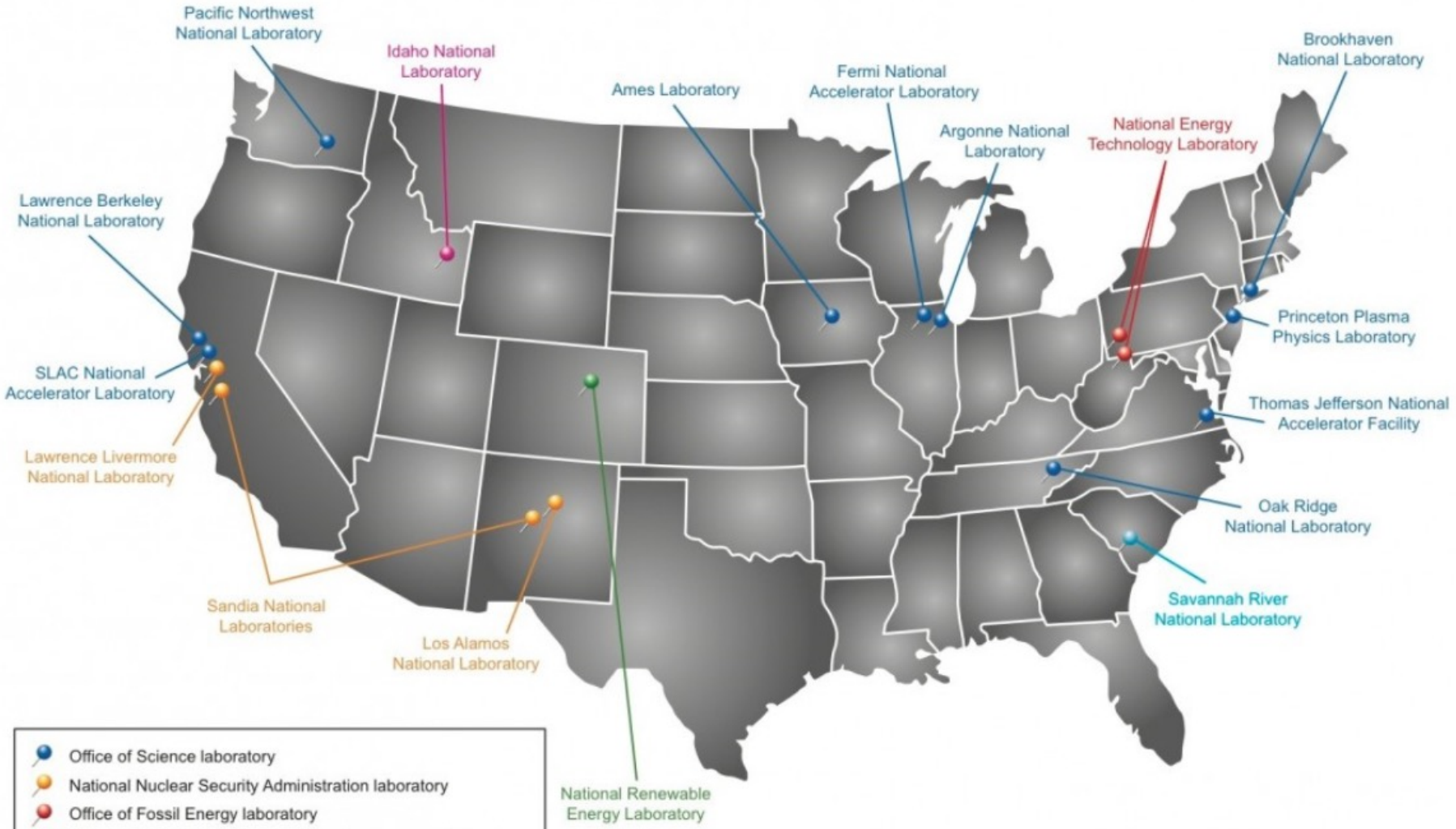
Friday

- The Machine Learning Begins...

Logistics

- Drivers, upon check-in will receive a placard to be displayed on the dashboard for the week.
- Adhere to speed limit postings, 30mph
- Building 438 Classroom – home base
- Attire: **must** wear long pants, flat closed-toe shoes and suggest you bring additional layers
- Personal devices (cell phones and laptops) are allowed
- BYO lunch or a few options available for purchase
  - Lunch break is typically from about 12:30pm to about 1:30pm
- Water refill stations located in building 438 and cafeteria

Department of Energy National Laboratories



Brookhaven National Laboratory

U.S. DEPARTMENT OF ENERGY

Brookhaven National Laboratory

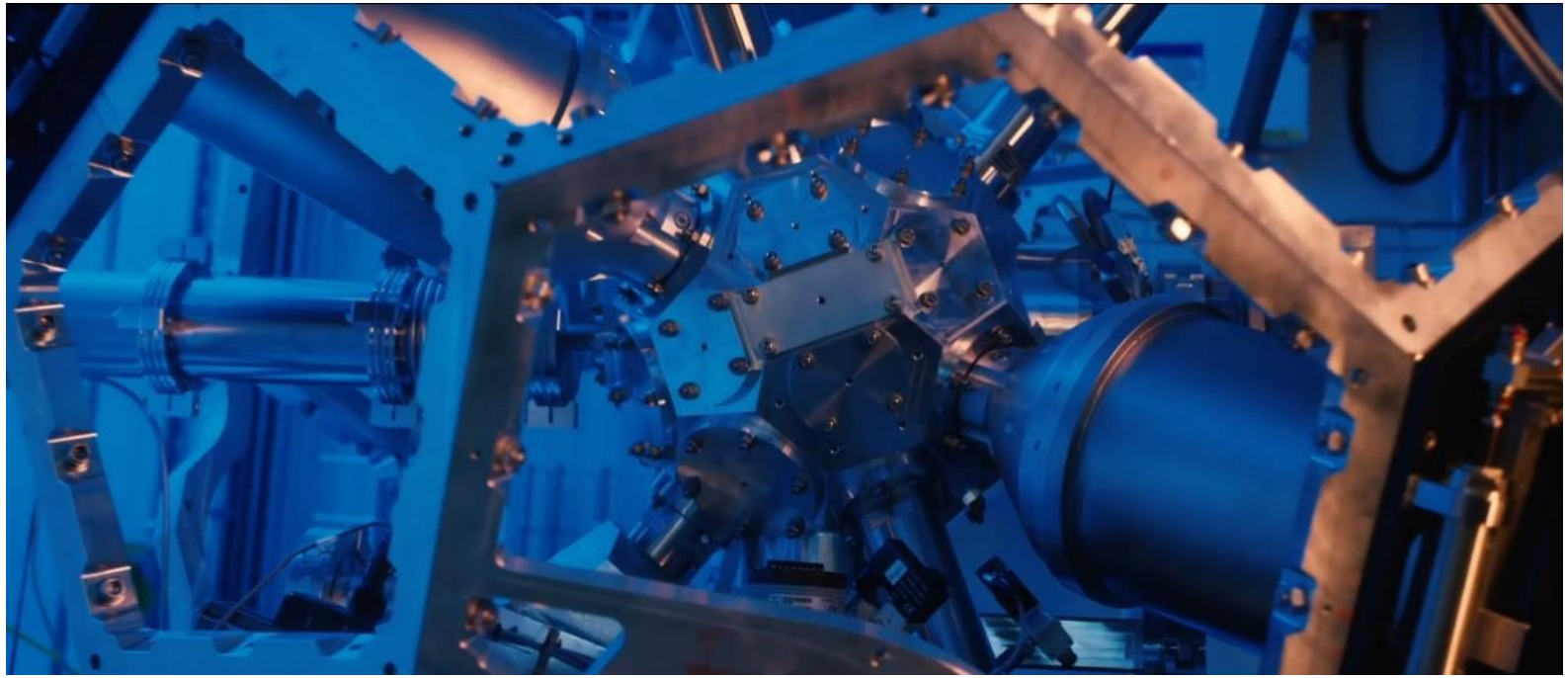
Our Vision: To accelerate pathways to scientific discovery and technological innovation that transform the world

Brookhaven National Laboratory

Our combination of facilities, people, and equipment gives us a unique and vital role in addressing national needs.

Brookhaven National Laboratory

About Brookhaven National Laboratory



YouTube Video - This is Brookhaven Lab

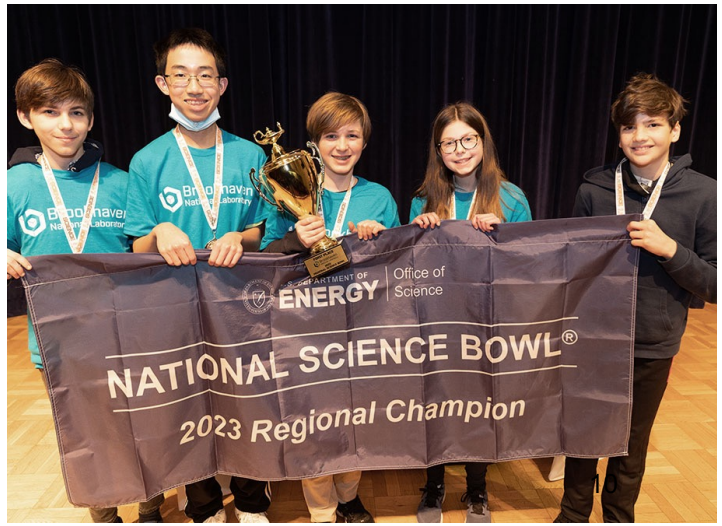
Preparing New Generations of STEM Professionals

Office of Educational Programs

Host ~30,000 students, interns, teachers and college faculty

Pre-College Programs

- Field trips
- Summer Programs
- Contests
- Teacher PD



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Preparing New Generations of STEM Professionals

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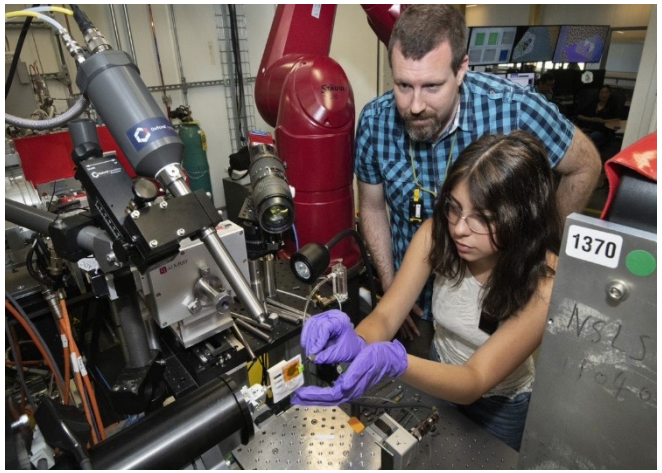
Pre-College Programs

- Open Space Stewardship
- High School Research Program
- SPARK



Brookhaven National Laboratory

Preparing New Generations of STEM Professionals

Office of Educational Programs

Host ~30,000 students, interns, teachers and college faculty

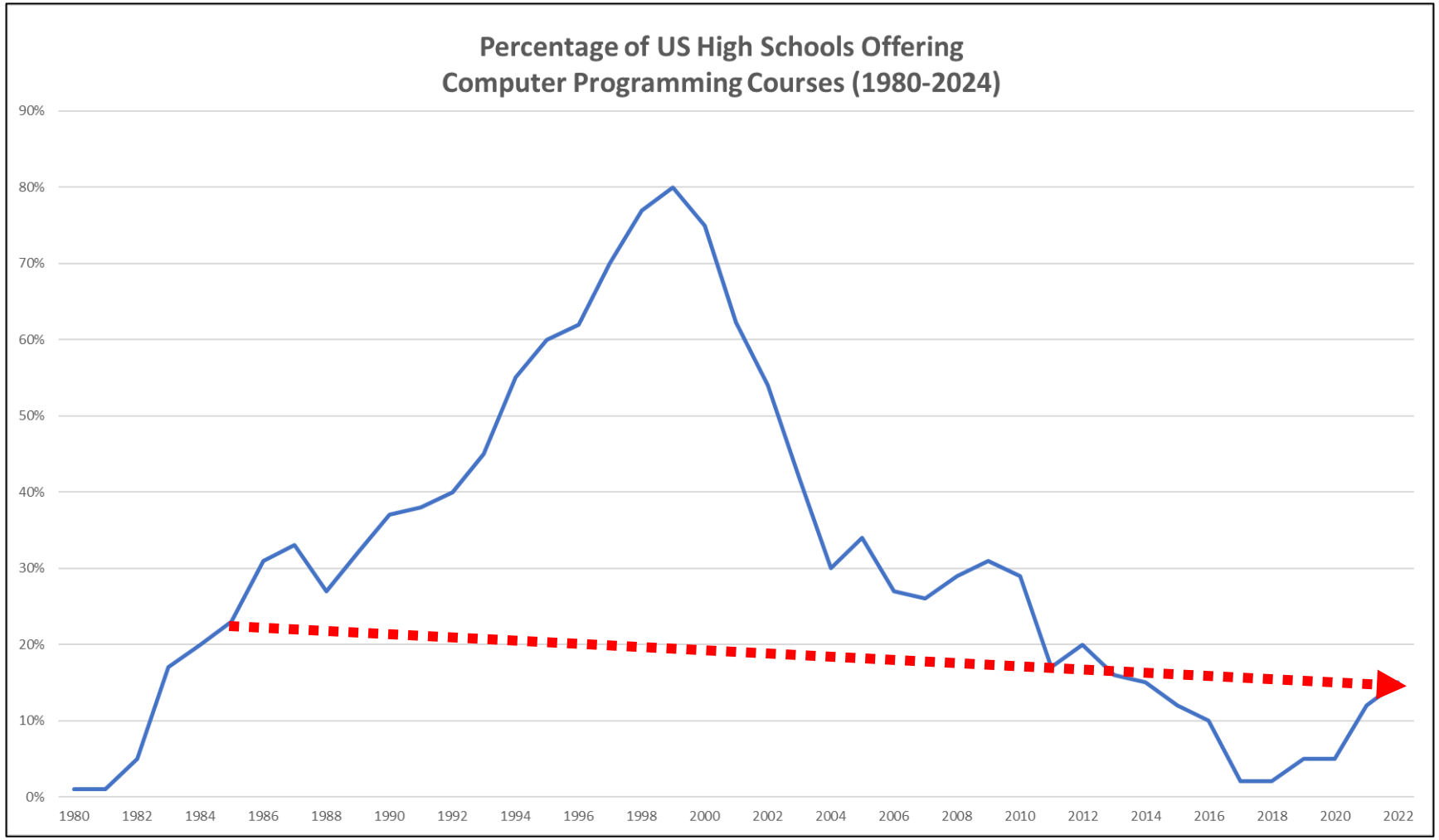
University and Faculty Programs

- College Internship Programs
- Visiting Faculty Program

There are research opportunities at all the DOE National Labs!

Brookhaven National Laboratory

A National Challenge



National Center for Education Statistics, US Dept. of Education

The Challenge to DOE

Scientists across DOE have noted a dramatic rise in the **startup latency** of interns who do not possess foundational programming skills

This latency means that for the ***initial 6-8 weeks of their assignment***, the interns are essentially unproductive as they must first acquire basic knowledge of how to write software

Instead of learning critical scientific principles from their mentor, the interns are spending their precious lab time **often working alone**, figuring out how to instruct the computer to perform rudimentary data processing tasks

From the perspective of DOE scientists, **the need to adeptly wield software tools has never been as urgent as it is today**

The Hype

Kevin's Story

Modern-day scientists and engineers are spending more and more of their work days in front of the computer. As an example, consider my friend Kevin, who works in oceanography and mechanical engineering. Whoa, sounds like he's probably spending all day out on high-tech boats rigging together mechanical devices like MacGyver and collecting data from underwater sensors, right? This must be his typical work day -- hard hats and heavy-duty work gloves.

The Reality

Actually, Kevin spends less than 5% of his time out on the ocean; the other 95% of the time, he's sitting in front of the computer writing programs to clean up, transform, process, and extract insights from data collected out in the field. This is what Kevin looks like at work on most days:

The same story plays out for scientists and engineers in all sorts of fields: astronomers, biologists, physicists, aerospace engineers, economists, geneticists, ecologists, environmental engineers, neuroscientists ... the list goes on and on. Modern-day science and engineering is all about processing, analyzing, and extracting insights from data.

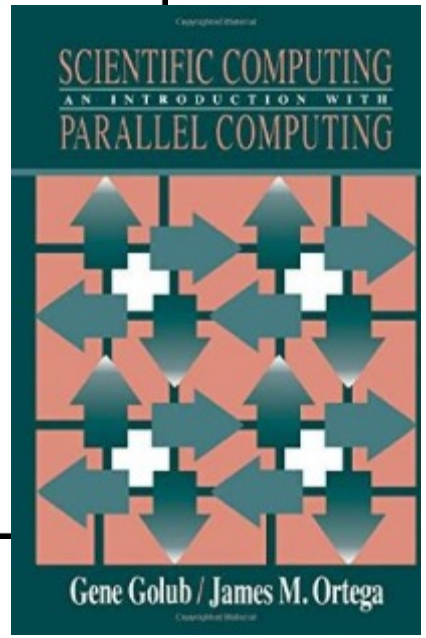
What is Scientific Computing?

Golub and Ortega: *"Scientific computing is the collection of tools, techniques and theories required to solve on a computer mathematical models of problems in science and engineering."*

Or a more narrow definition: *"Development and use of numerical methods and mathematical models to solve real-world problems efficiently on computers."*

Interdisciplinary field requiring:

- knowledge about the underlying (physical) problem,
- ability to formulate a mathematical model,
- stable & accurate numerical schemes,
- efficient implementation on high performance computers.



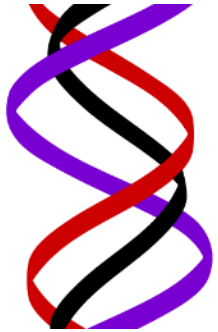
What is Scientific Computing?

Scientific computing problems **cannot be solved** using just a graphing calculator or a spreadsheet program

- A computer should not be viewed as just another closed-form benchtop instrument with fixed functionality
- SciComp does not require writing thousands of lines of code to answer problems – complete code usually fits on **one** slide!

SciComp is **applied** computer science

- The first name of CompSci is *computer*
- The first name of SciComp is **science**
- A **triple helix** of math, science, and computin



SciComp vs CompSci

Scientific Computing

- Probability and Statistics
- Simulation and Modelling
- Data Visualization
- Storing and Analyzing Very Large Datasets
- Parallel & Distributed Algorithms
- Speed and Accuracy Paramount
- Functional Languages
- Open-Ended Problems with Unknown Solutions

Computer Science

- General Data Structures
- Design Methodologies
- Procedural Languages
- Stand-Alone Programs
- Emphasis on Object-Orientation
- Simple Data Models
- Sequential Algorithms
- Less Graphics Intensive
- Directed Closed-Form Problems with Known Solutions

SciComp = Just Enough CompSci

Data **types**: int, float, bool, string

Data **structures**: lists, arrays, dictionaries, classes, modules

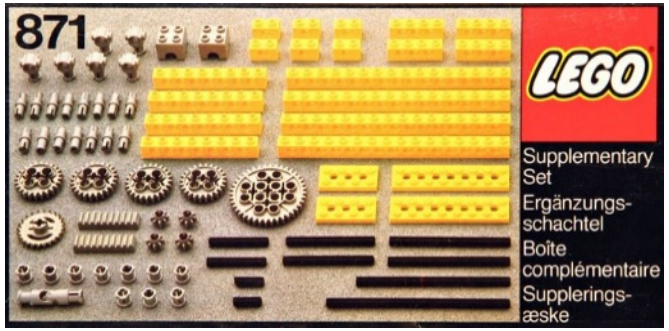
Functions: def, return

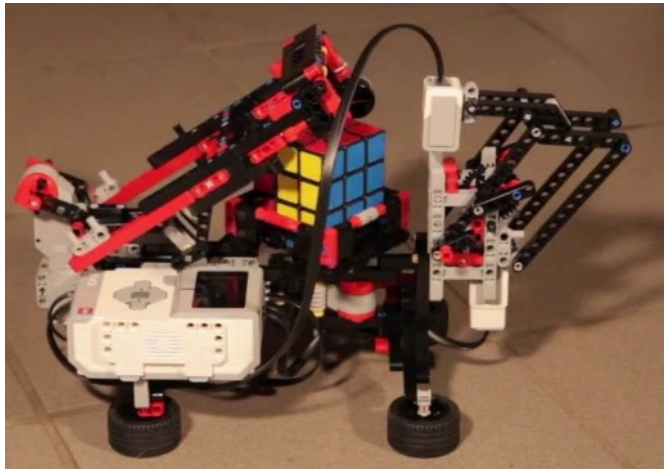
Statements: if, for, while, break

Patterns: vectorization, divide & conquer, list comprehensions

Algorithms: GCD, mean/variance, sorting, searching

Modules: numpy, matplotlib, numba, scipy, sympy, scikit-learn





SciComp As Translational Science

"The algorithm that almost won the cold war"

$$u(\mathbf{x}) = \begin{cases} \dfrac{\sum_{i=1}^{N} w_i(\mathbf{x}) u_i}{\sum_{i=1}^{N} w_i(\mathbf{x})}, & \text{if } d(\mathbf{x}, \mathbf{x}_i) \neq 0 \text{ for all } i \\ u_i, & \text{if } d(\mathbf{x}, \mathbf{x}_i) = 0 \text{ for some } i \end{cases}$$

where

$$w_i(\mathbf{x}) = \frac{1}{d(\mathbf{x}, \mathbf{x}_i)^p}$$

```python
def calc_idw_height(xi, yi, p):
    sum_weight = 0.0
    sum_height_weight = 0.0
    for si in range(num_samples):
        distance = np.hypot(grid_x[xi, xi] - samples_x[si],
                            grid_y[yi, yi] - samples_y[si])
        if distance == 0:
            return samples_z[si]
        weight = 1 / np.power(distance, p)
        sum_weight += weight
        sum_height_weight += samples_z[si] * weight
    return sum_height_weight / sum_weight
```

11 lines of code can change the world!

SciComp is the ability to translate mathematical expressions of scientific concepts into correct and efficient software code

US Department of Labor - 2019

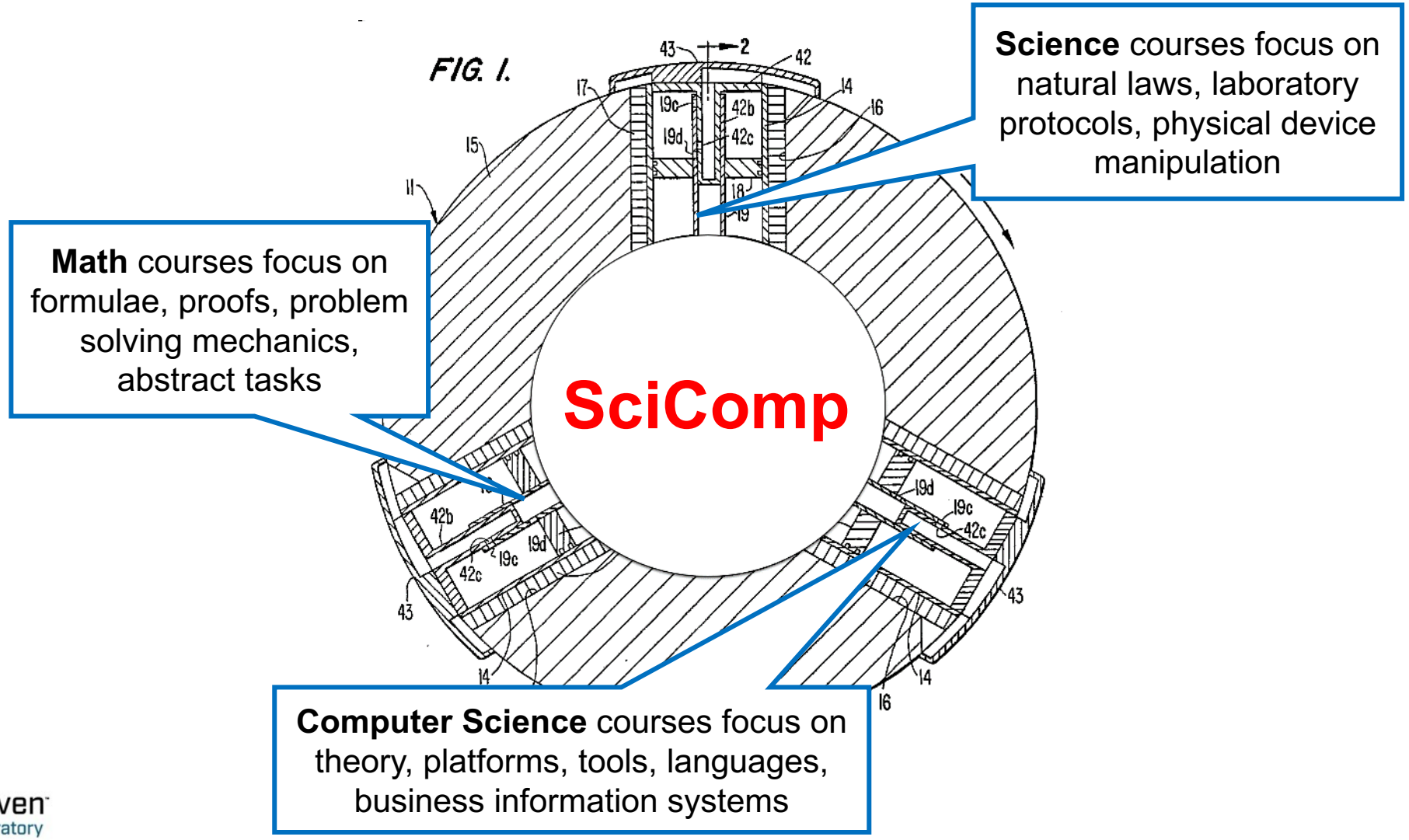
Robotics Engineering Careers

Quick Facts: Electro-mechanical Technicians	
2018 Median Pay	$57,790 per year $27.78 per hour
Typical Entry-Level Education	Associate's degree
Work Experience in a Related Occupation	None
On-the-job Training	None
Number of Jobs, 2016	13,800
Job Outlook, 2016-26	4% (Slower than average)
Employment Change, 2016-26	500

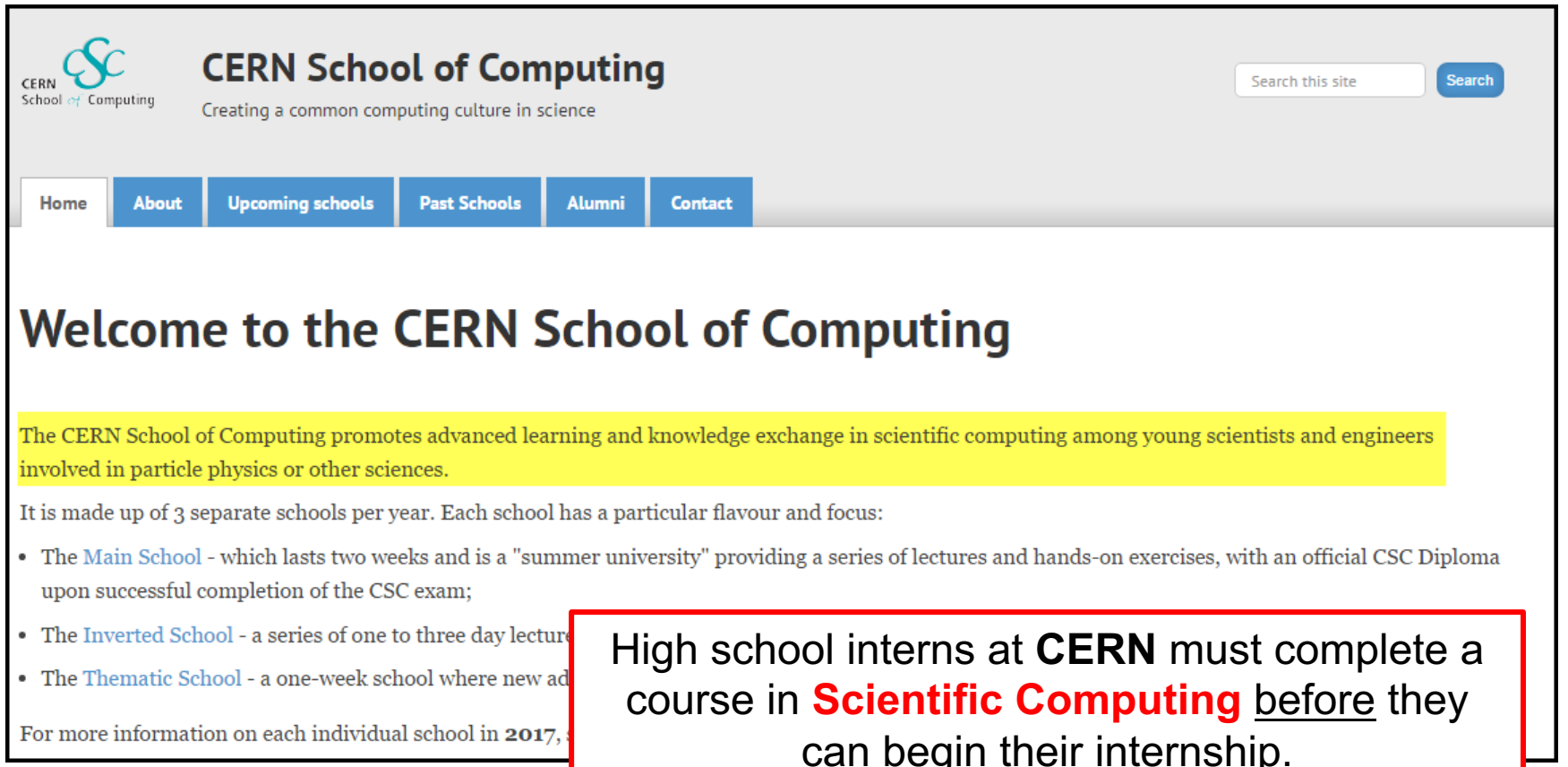
Scientific Computing Careers

Quick Facts: Computer and Information Research Scientists	
2018 Median Pay	$118,370 per year $56.91 per hour
Typical Entry-Level Education	Master's degree
Work Experience in a Related Occupation	None
On-the-job Training	None
Number of Jobs, 2016	27,900
Job Outlook, 2016-26	19% (Much faster than average)
Employment Change, 2016-26	5,400

SciComp Is Getting Lost in the Middle



SciComp = The Pathway to Internships



CERN School of Computing

Creating a common computing culture in science

Search this site | Search

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Welcome to the CERN School of Computing

The CERN School of Computing promotes advanced learning and knowledge exchange in scientific computing among young scientists and engineers involved in particle physics or other sciences.

It is made up of 3 separate schools per year. Each school has a particular flavour and focus:

- The Main School - which lasts two weeks and is a "summer university" providing a series of lectures and hands-on exercises, with an official CSC Diploma upon successful completion of the CSC exam;
- The Inverted School - a series of one to three day lectur
- The Thematic School - a one-week school where new ad

For more information on each individual school in **2017**,

High school interns at **CERN** must complete a course in **Scientific Computing** before they can begin their internship.

That is how important CERN views these skills!

Scientific Computing with Python

Python is quickly becoming one of the **most heavily used languages** in science projects

Python runs on all major modern **operating systems** and is completely free and open-source (not vendor controlled)

Python makes it easy for your code to directly integrate with a large spectrum of available 3rd party software

Python code runs **consistently** on different platforms and scales well from small IoT devices to large server clusters

Python benefits from a very active and growing user community that continues to enhance the language

Useful Python Reference Sites

https://colab.google

https://docs.python.org/3/tutorial

https://www.learnpython.org

https://realpython.com

https://www.w3schools.com/python

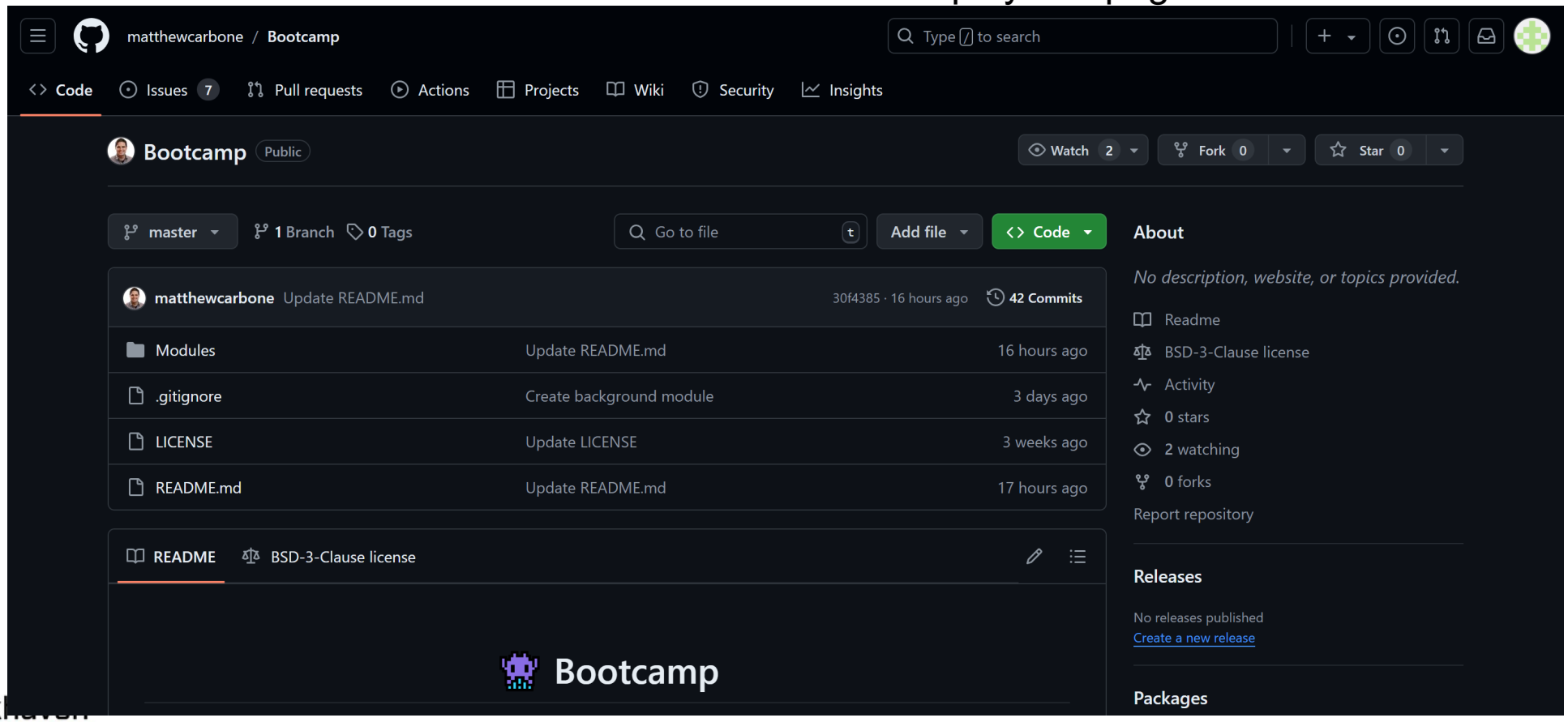
https://www.fullstackpython.com

Bookmark It!

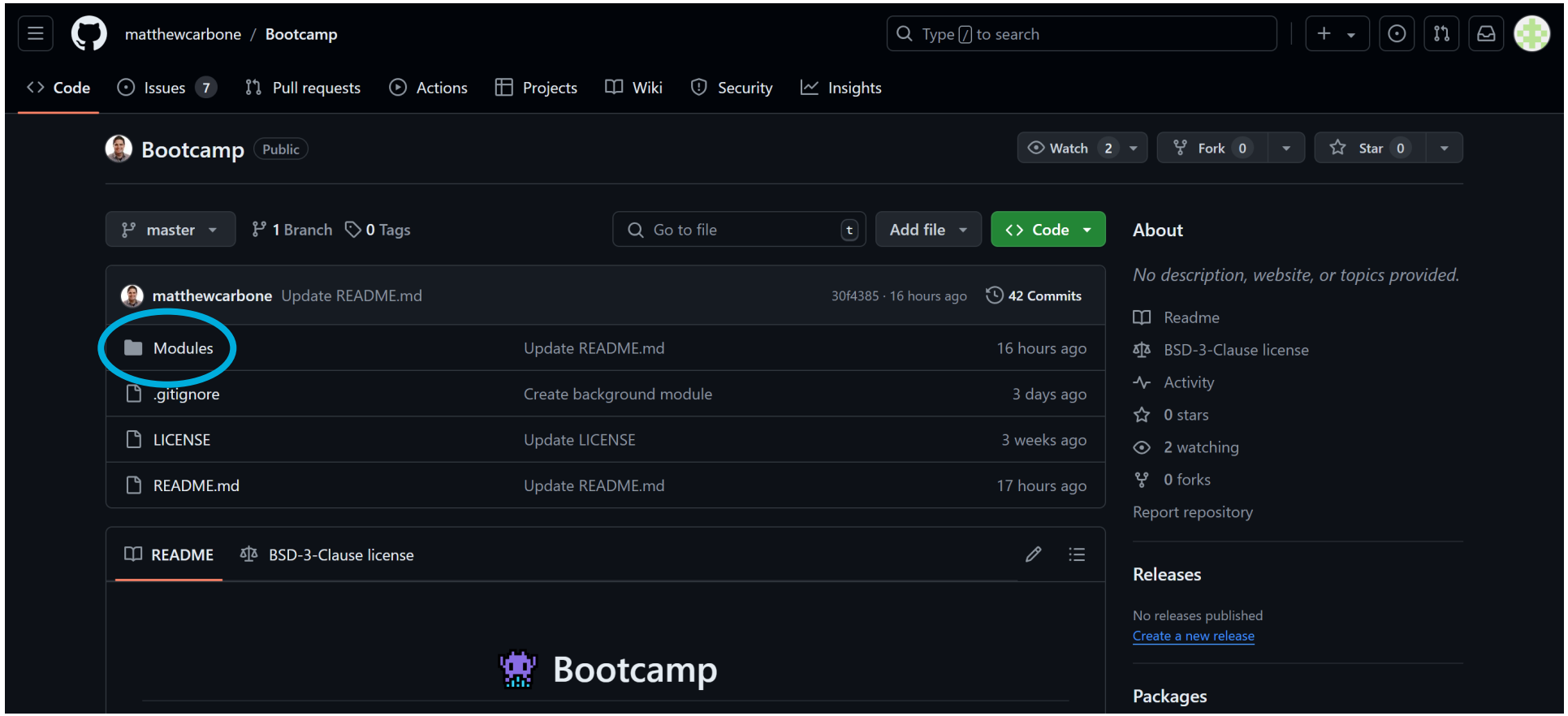
Access the Courseware – Step 1

Go to this link: https://github.com/matthewcarbone/Bootcamp

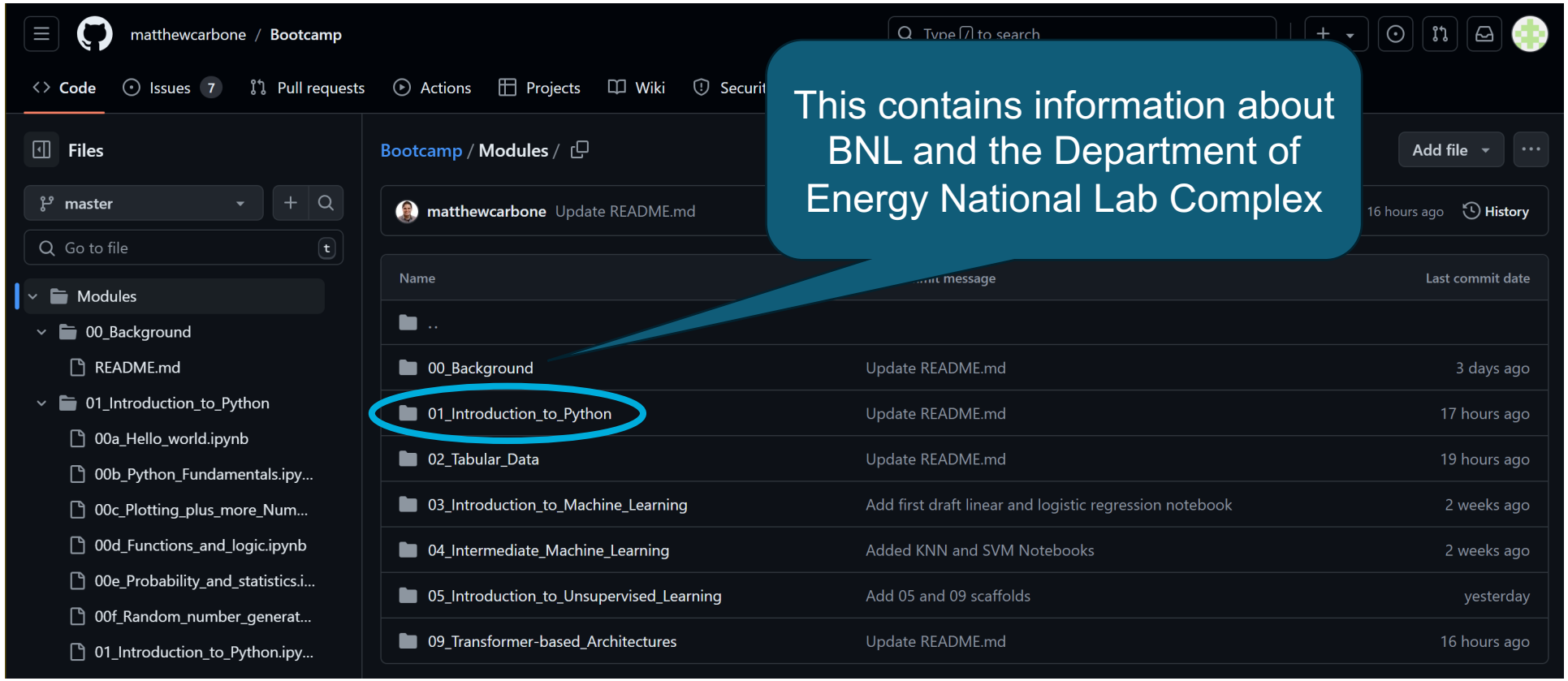
Your web browser should then display this page:



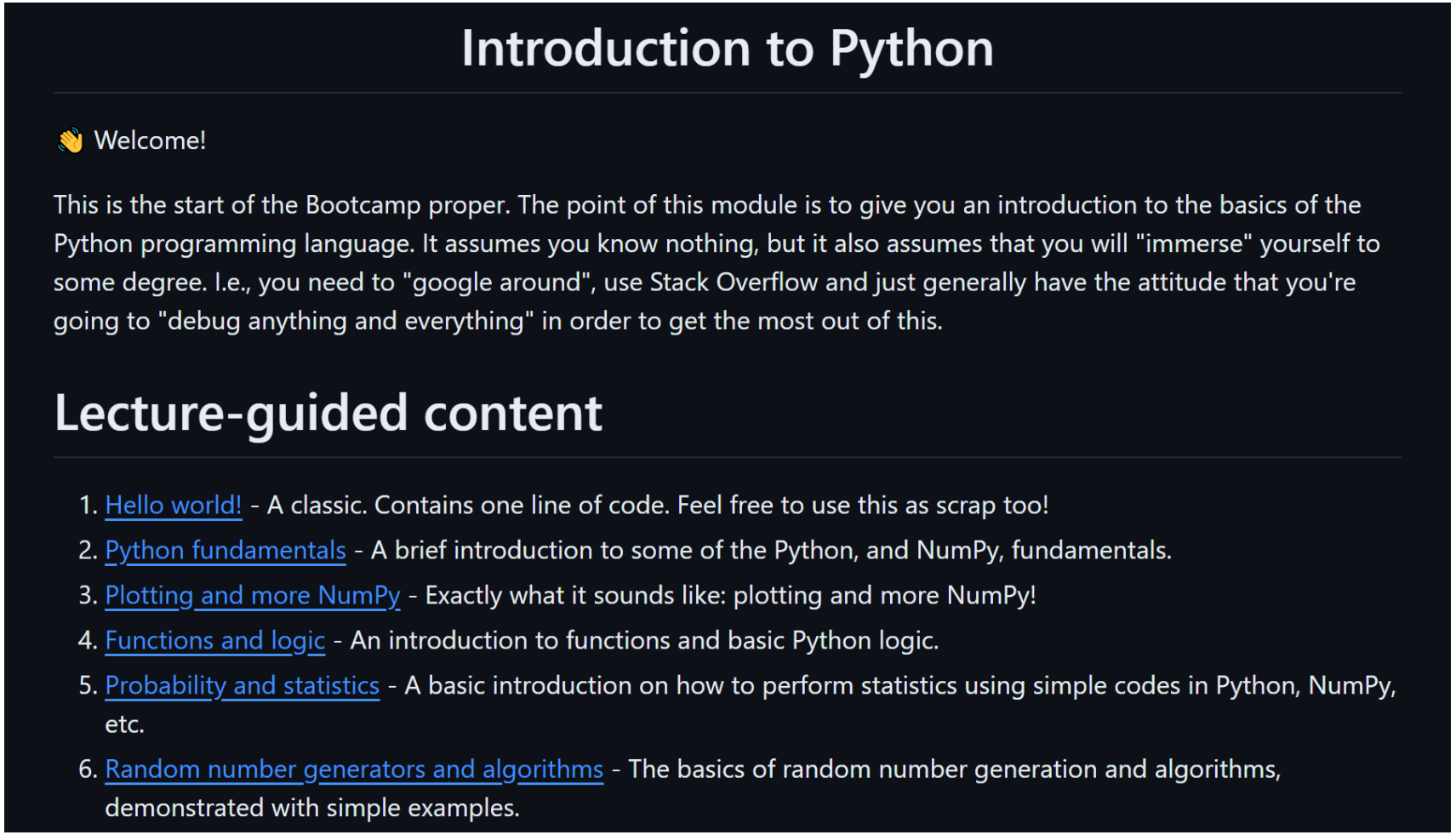
Get the Courseware – Step 2



Get the Courseware – Step 3



Get the Courseware – Step 4



Introduction to Python

👋 Welcome!

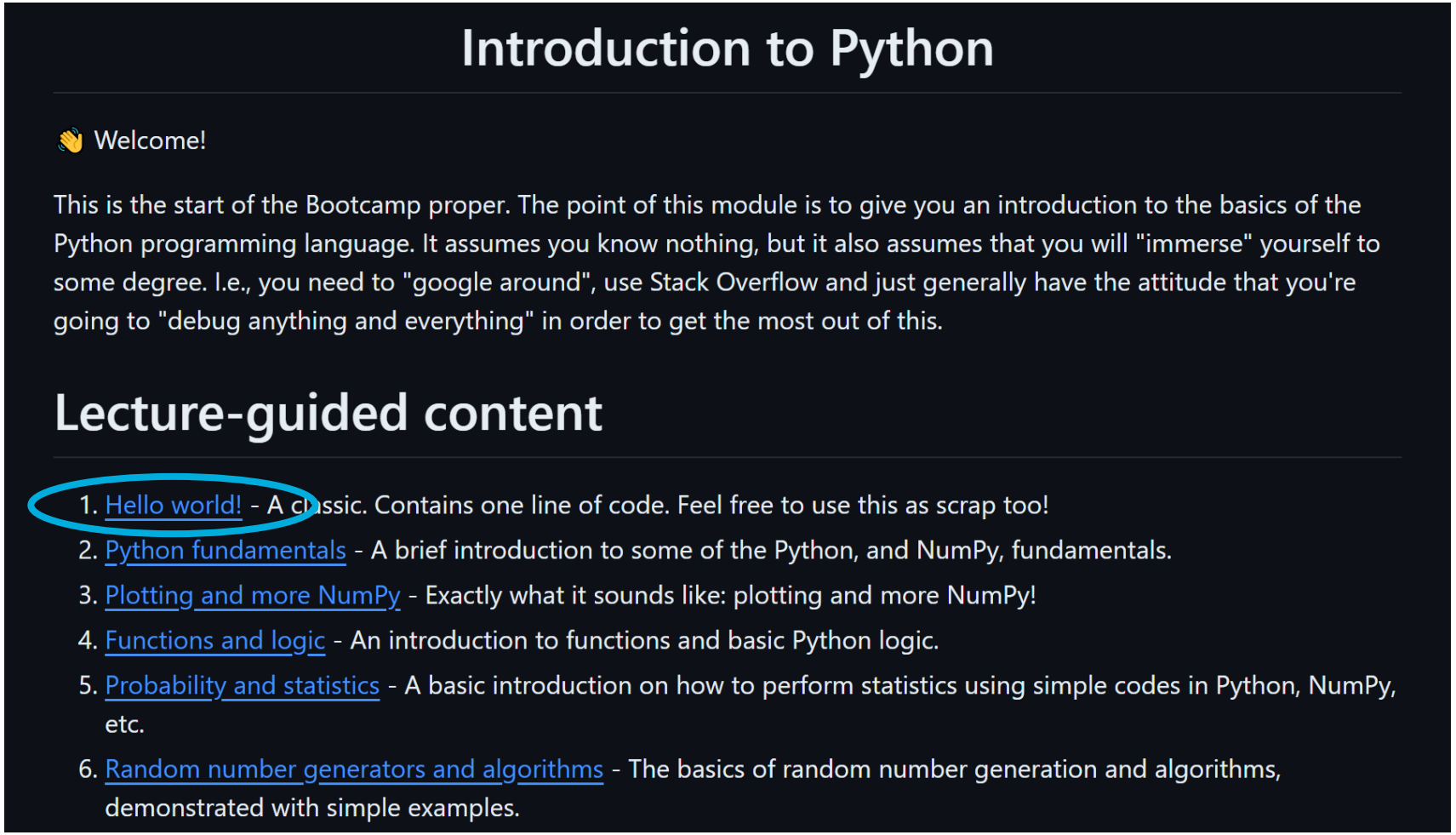
This is the start of the Bootcamp proper. The point of this module is to give you an introduction to the basics of the Python programming language. It assumes you know nothing, but it also assumes that you will "immerse" yourself to some degree. I.e., you need to "google around", use Stack Overflow and just generally have the attitude that you're going to "debug anything and everything" in order to get the most out of this.

Lecture-guided content

1. Hello world! - A classic. Contains one line of code. Feel free to use this as scrap too!
2. Python fundamentals - A brief introduction to some of the Python, and NumPy, fundamentals.
3. Plotting and more NumPy - Exactly what it sounds like: plotting and more NumPy!
4. Functions and logic - An introduction to functions and basic Python logic.
5. Probability and statistics - A basic introduction on how to perform statistics using simple codes in Python, NumPy, etc.
6. Random number generators and algorithms - The basics of random number generation and algorithms, demonstrated with simple examples.

Scroll down to get to this content

Open hello_world.ipynb



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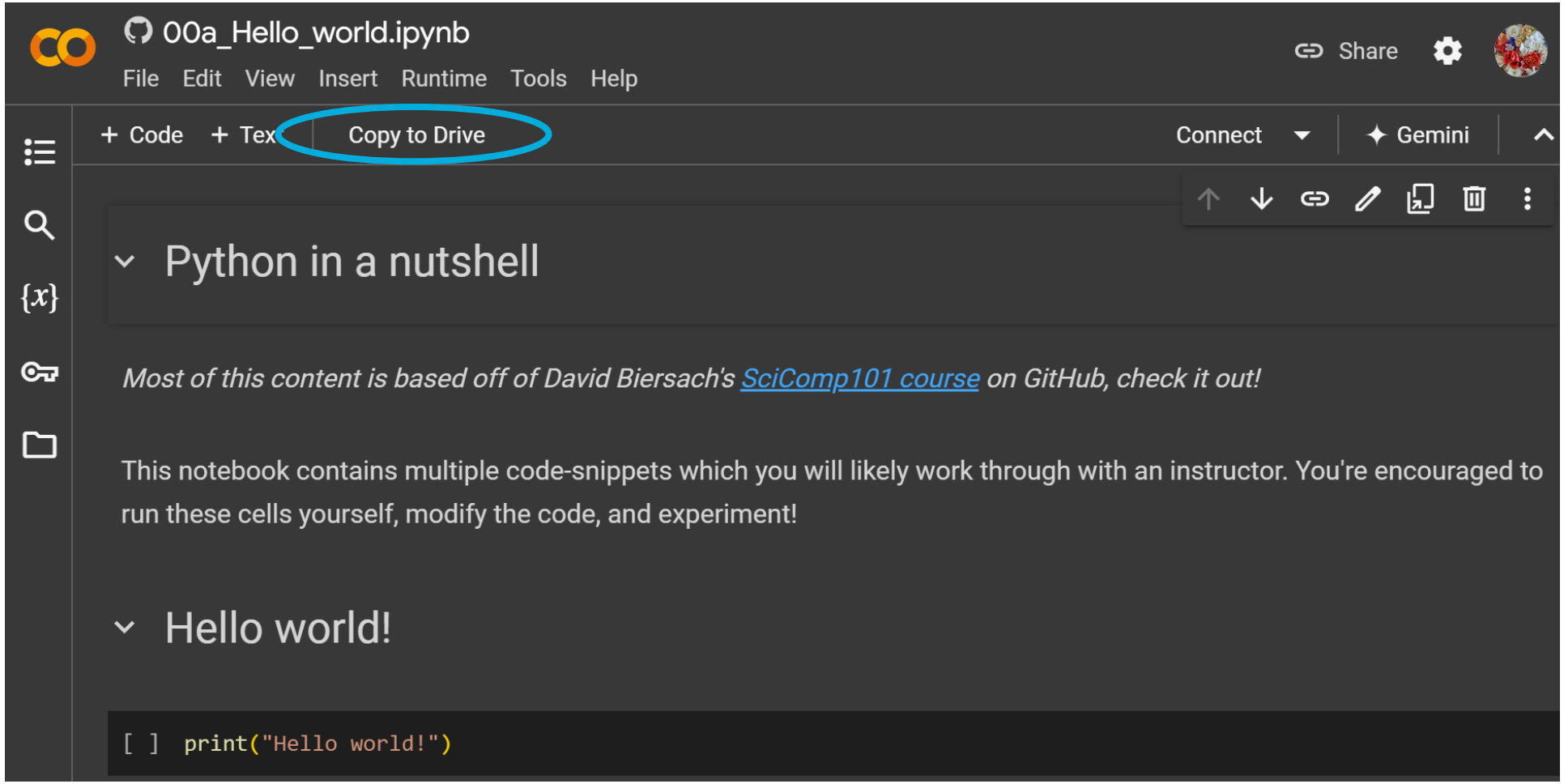
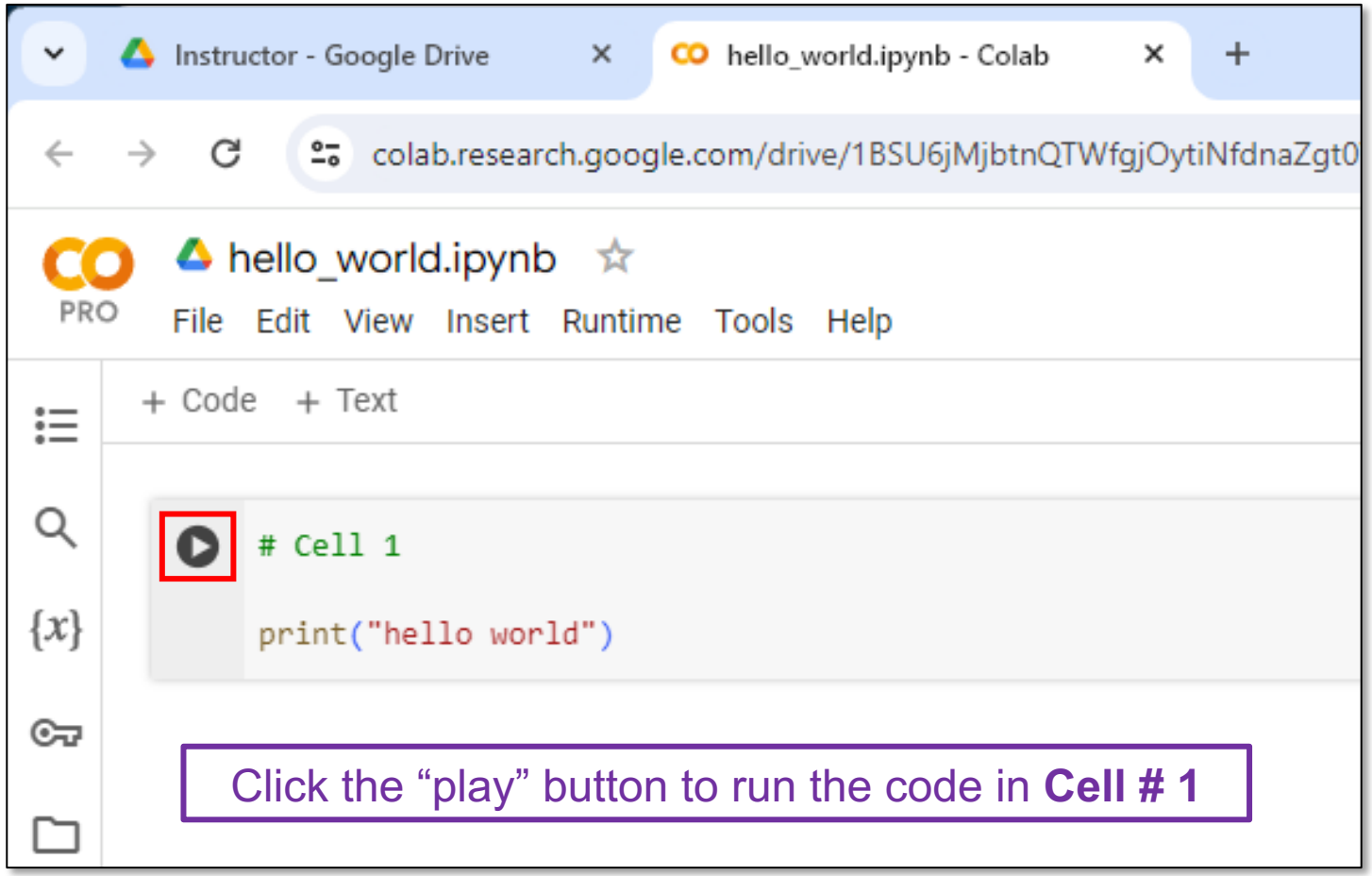
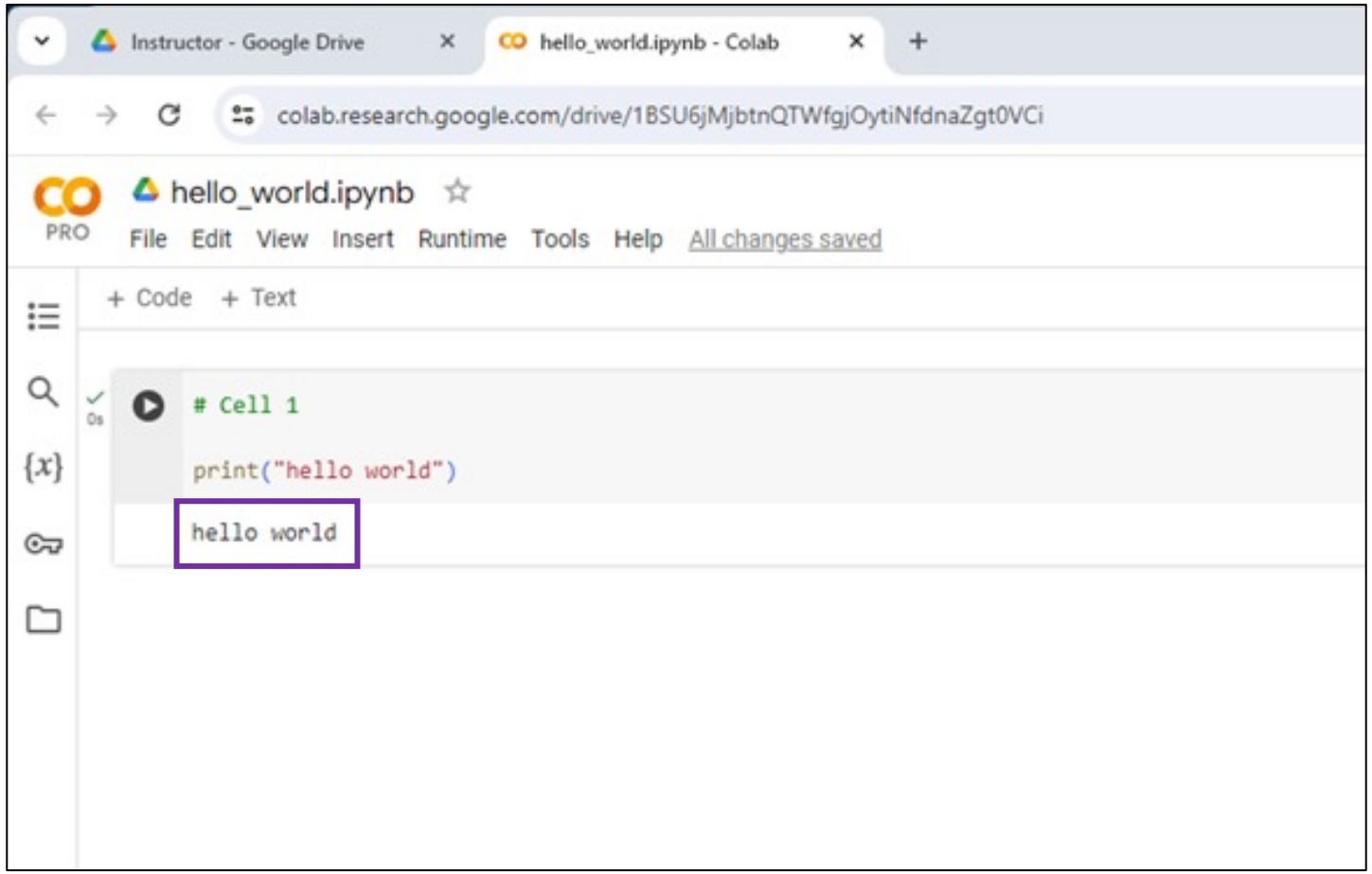
Make Your Own Copy



Run hello_world.ipynb



Check hello_world.ipynb



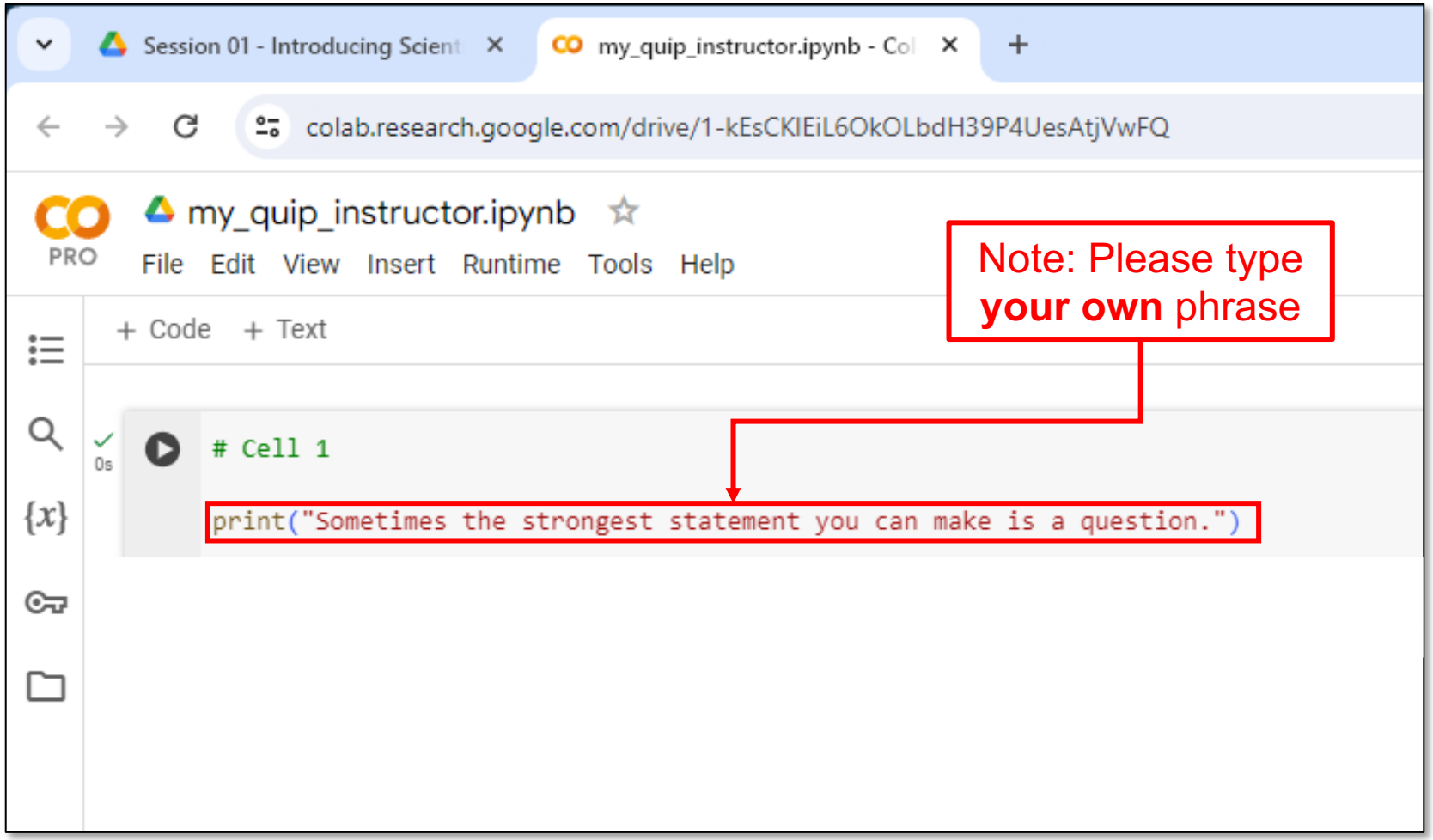
Session 01 – Know You Know…

- Scientific Computing **is not the same** as Computer Science
- You cannot do modern science without knowing how to **program** a computer (not just *use* a computer)
- The US Department of Energy offers high school and college internships at 17 National Laboratories across the USA
- One of the best ways to **differentiate yourself** from other students competing for internships is to develop foundational skills in scientific computing
- AP College Board is now offering AP exams in **Python**
- Google **Colab** is a cost-free cloud-hosted service built on Python Notebooks that works with Google **Drive**

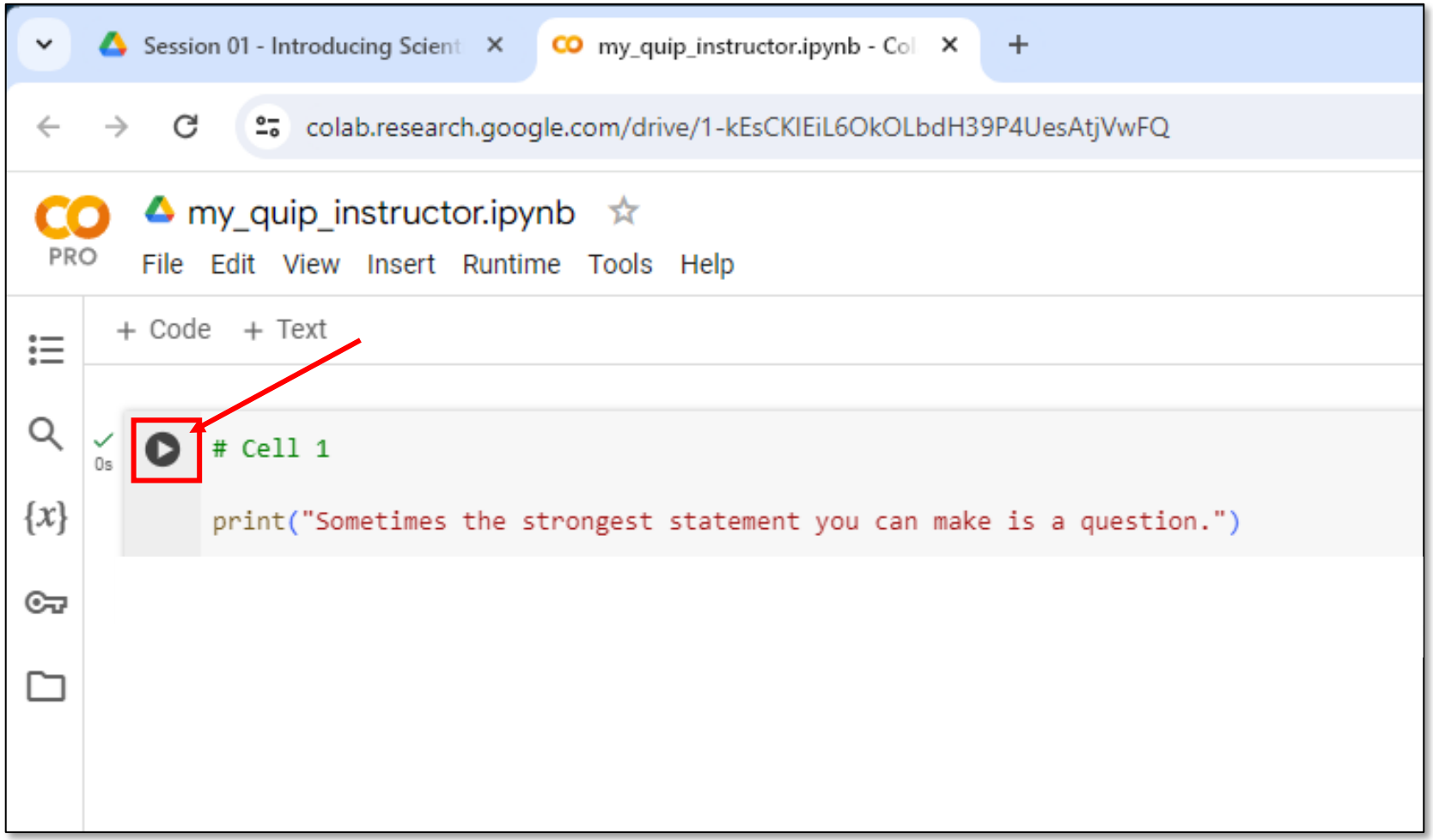
TASK 01

Add to your “Hello World” code to make it also display a quip of your choosing or creation

How Do I Do That?



Run my_quip.py



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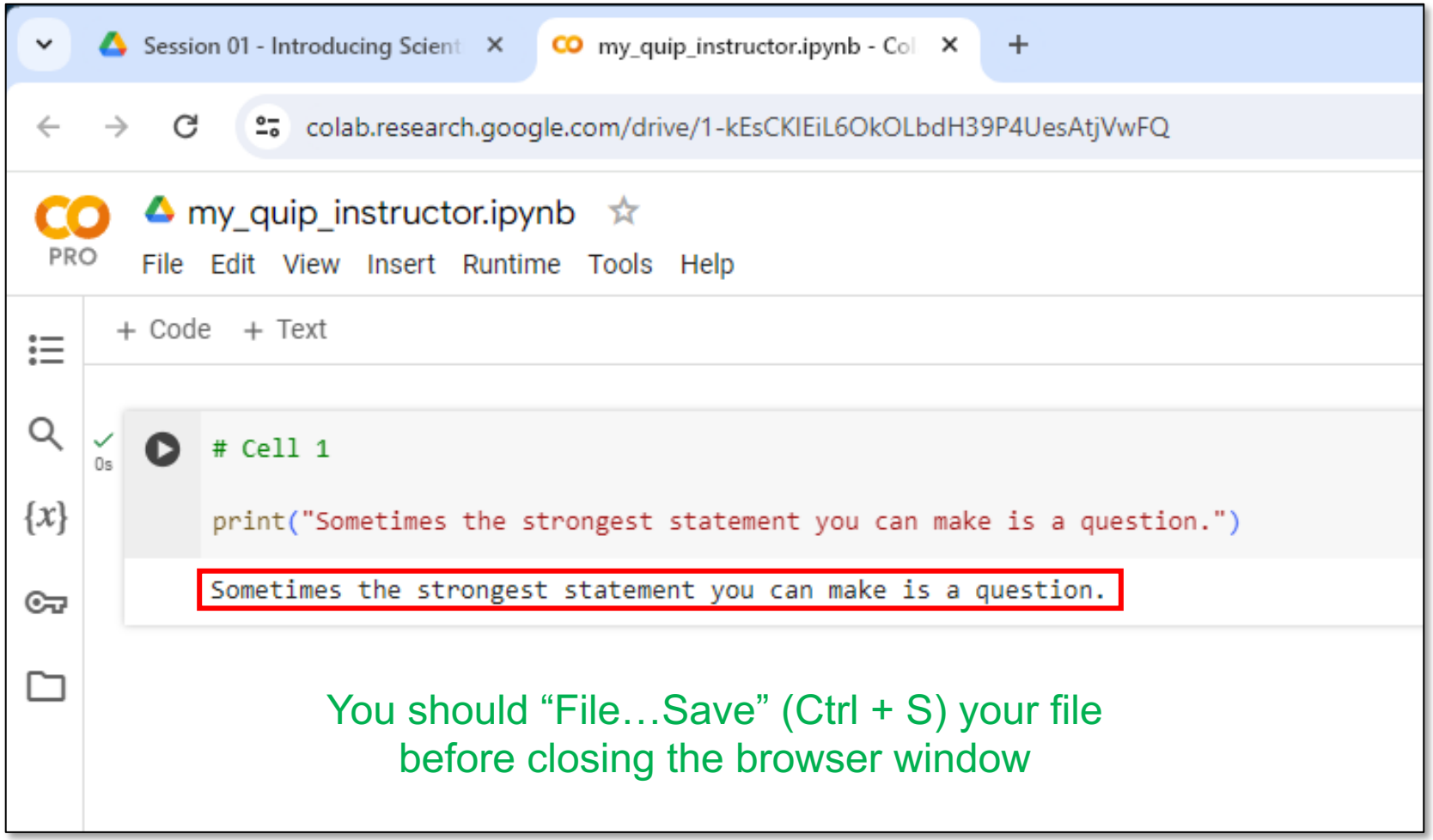

You should “File…Save” (Ctrl + S) your file
before closing the browser window