UNIVERSITY OF TORONTO

PSCB57
Introduction to Scientific Computing

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Outline of today’s lecture

Scientific Computing

What you will learn and what not.

PSCB57

Lecture style, tutorials, assignments, tests, marks

Python

Introduction

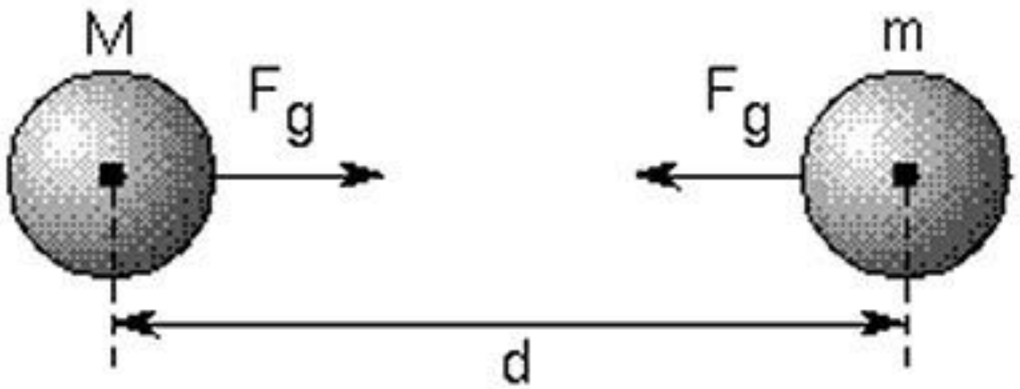
Welcome to Scientific Computing

Why do we need scientific computing?

Complexity

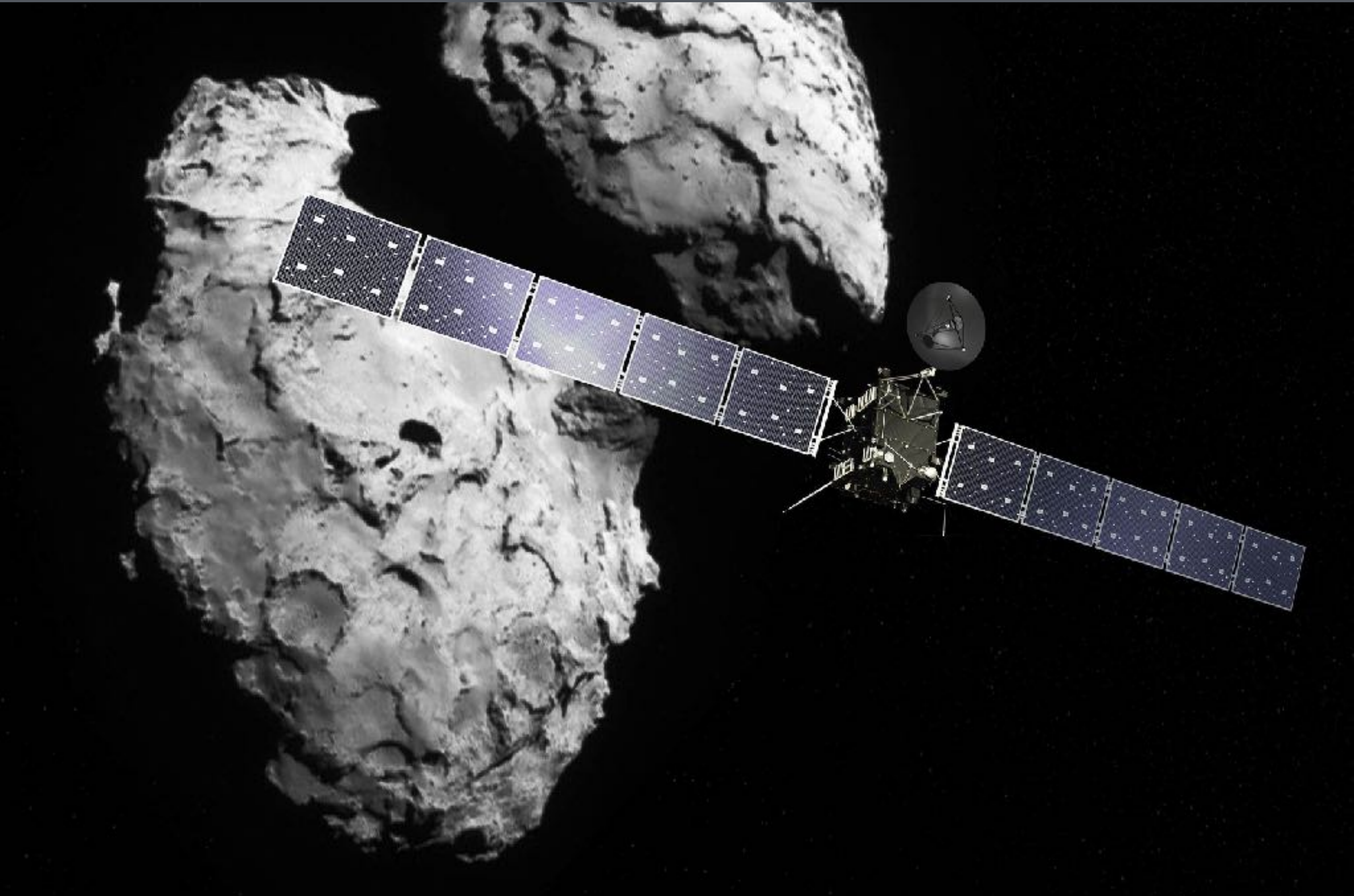
In school/university, you learn the basic fundamental laws. Examples are easy. You do them with pen and paper. Real life is more complicated.

How you learn physics in school/university



$$F_g = \frac{GMm}{d^2}$$

If you do science, it’s more complicated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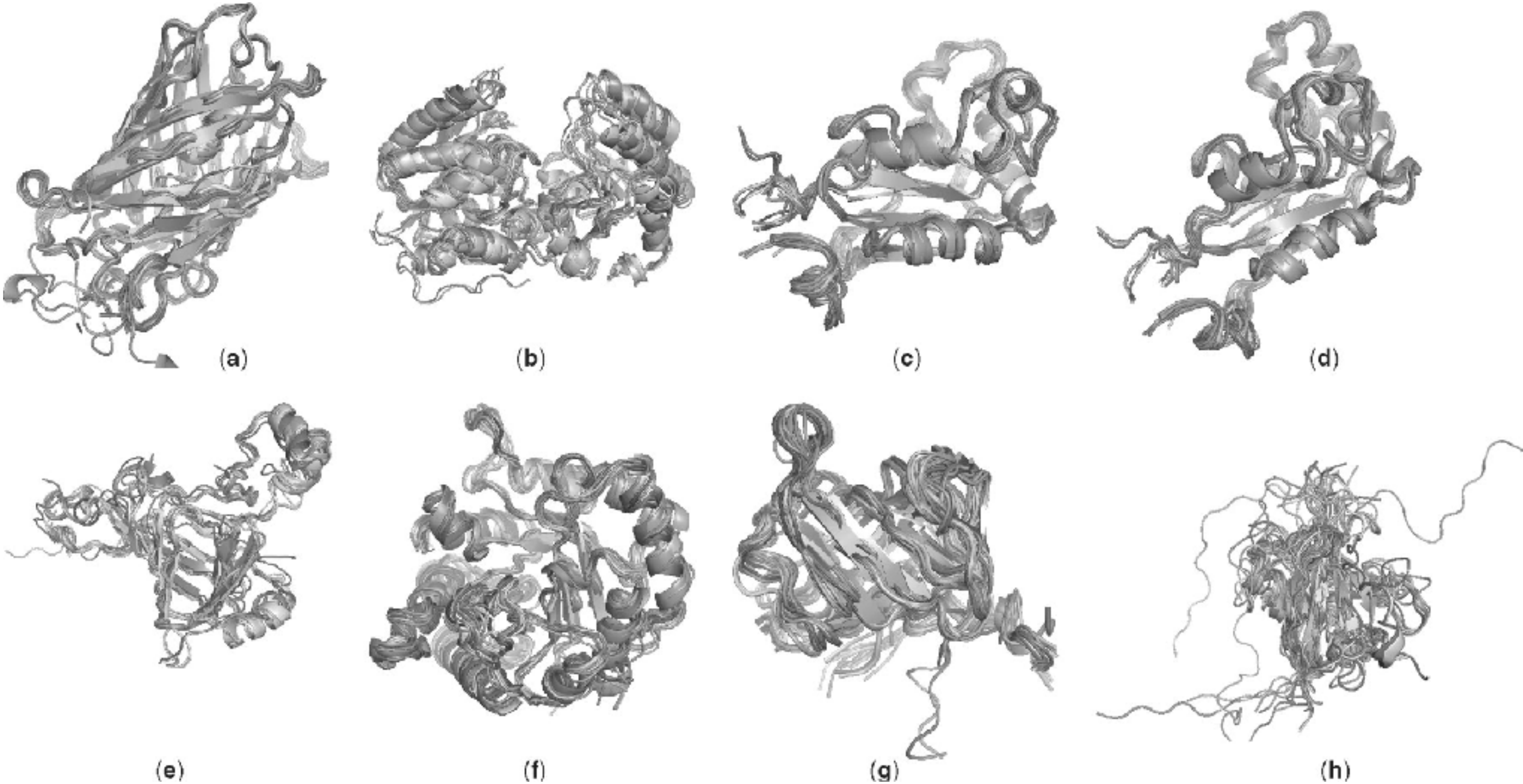
Chemistry



Why do we need scientific computing?

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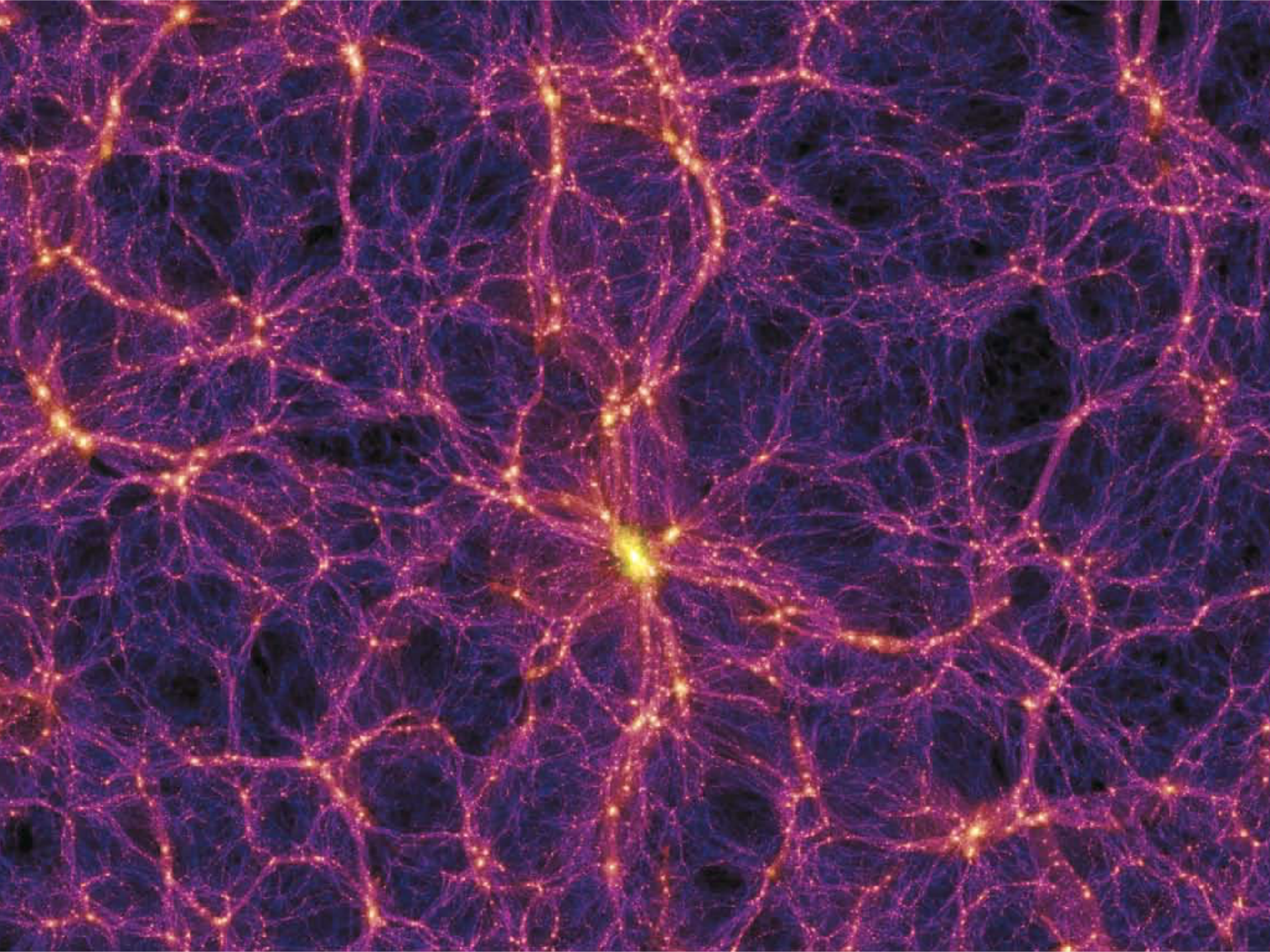
Simulations

To proof a new theory, you need to make testable predictions. Often, it is not possible to test the predictions in an experiment. Thus, we run simulations.



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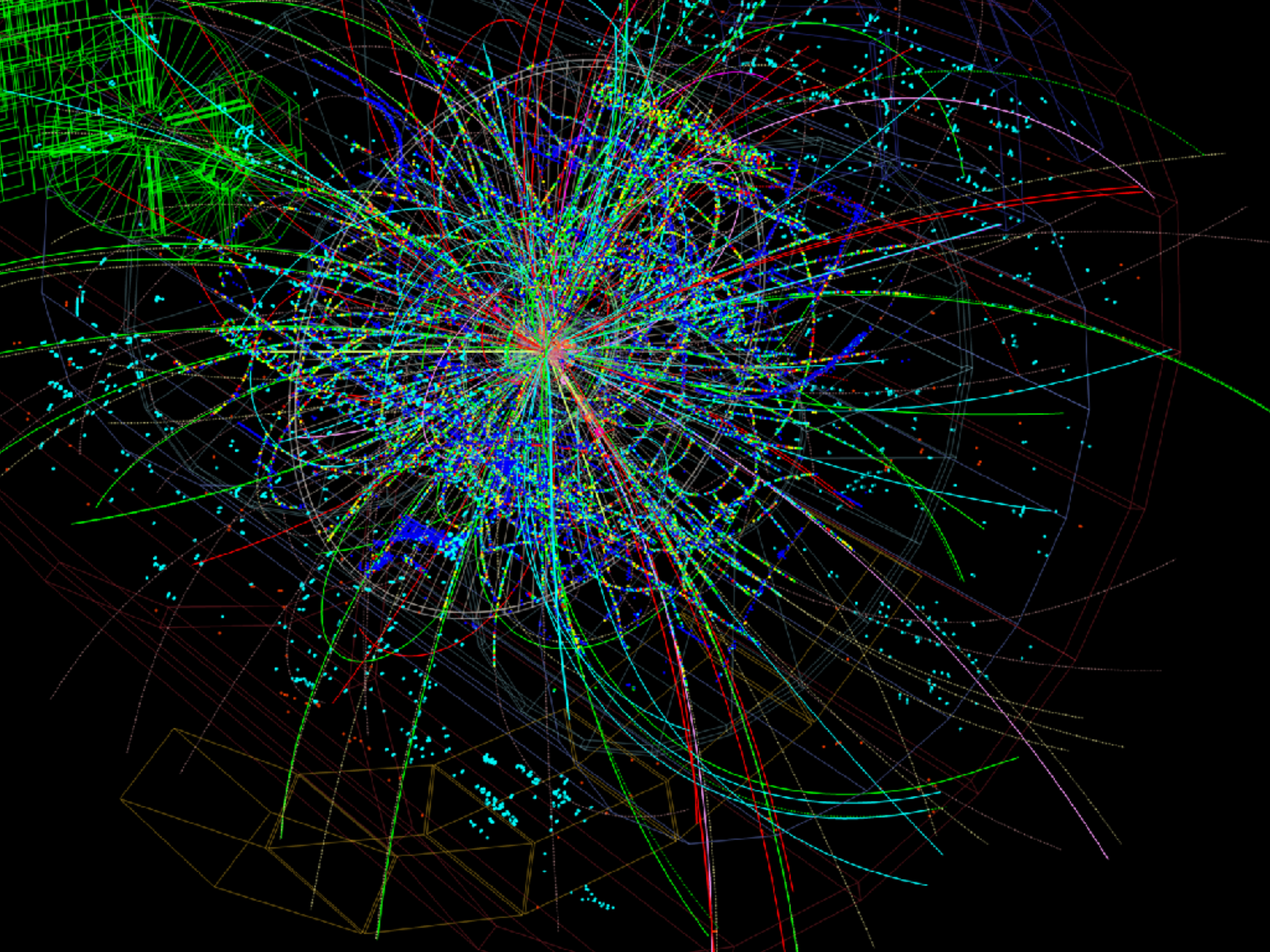
Data analysis

Often experiments create a huge amount of data. Analyzing data can be very challenging. Visualization help understand data.



Skills, tools needed for scientific computing

Mathematics

You need to be able to formulate the question you have in mathematical terms.

Discretization

Computers can store only a finite amount of information. You often have to discretize the system you’re interested in.

Programming

You need to be able to tell the computer precisely what to do.

Skills, tools needed for scientific computing

Mathematics

You need to be able to formulate the question you have in mathematical terms.

—> Prerequisite

—> PSCB57 (Differential Equations Introduction)

Discretization

Computers can store only a finite amount of information. You often have to discretize the system you're interested in.

—> PSCB57

Programming

You need to be able to tell the computer precisely what to do.

—> Some previous programming experience helps

—> You'll learn how to apply your knowledge in PSCB57

Skills, tools needed for scientific computing

Mathematics

Linear algebra, vectors, matrices, linear systems of equations, integration, differentiation, ordinary differential equations.

Discretization

Binary representation, floating point numbers, finite precision, root finding methods, finite differencing, numerical integration, time and space discretization for differential equations

Programming

Python, Jupyter Notebooks, numerical scalings, big O notation, visualization, working with large dataset, using numerical packages, parallelization and high performance computing

PSCB57

Lectures

Ask questions

Take notes

Be on time

Short break after 50 minutes

No 📱

No 🥘

Assignments

Total of 5 assignments, difficulty varies

Submit via Quercus

I highly recommend to test your submission

Typically, you have to pass a test in next tutorial

Software

You have to be able to run python3 code and Jupyter Notebooks.

1. Use your own computer. Linux, Mac, or Windows are fine. For Windows/Mac, install anaconda.

2. Use computers in physics labs (SW5). You can use these whenever there is no other tutorial/lab scheduled.

Python

Why python?

- Becoming more and more popular for data intensive computations in science
- Easy to learn
- High level language
- Freely available
- Extensive libraries

Python is dynamically-typed

```
employeeName = 9
employeeName = "Steve Ferg"
```

Python is not fast

- Python is run in an interpreter
- Not compiled down to machine code
- Typically, the most computationally expensive parts are written in C
- Python is used to call that code

Python

- You don’t need to be an expert.
- Know enough so that you are able to google what you don’t know.
- The assignments will give you a guide as to what is required for this course.

Python Introduction