



# PSCB57

# Introduction to Scientific

# Computing

Prof. Hanno Rein

Outline of today's lecture

# Scientific Computing

What you will learn and what not.

## PSCB57

Lecture style, tutorials, assignments, tests, marks

## Python

Why python, what you should know by now and what not.

## Number representations

Integers, floating point numbers

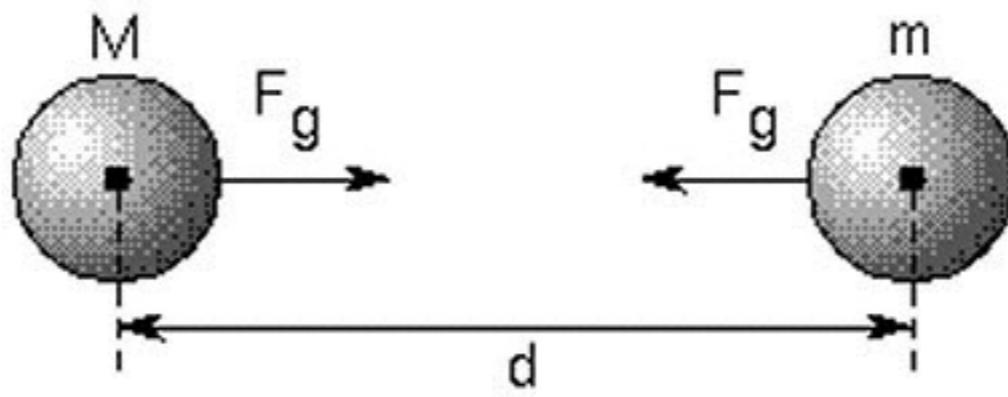
# Scientific Computing

# Why do we need scientific computing?

## Complexity

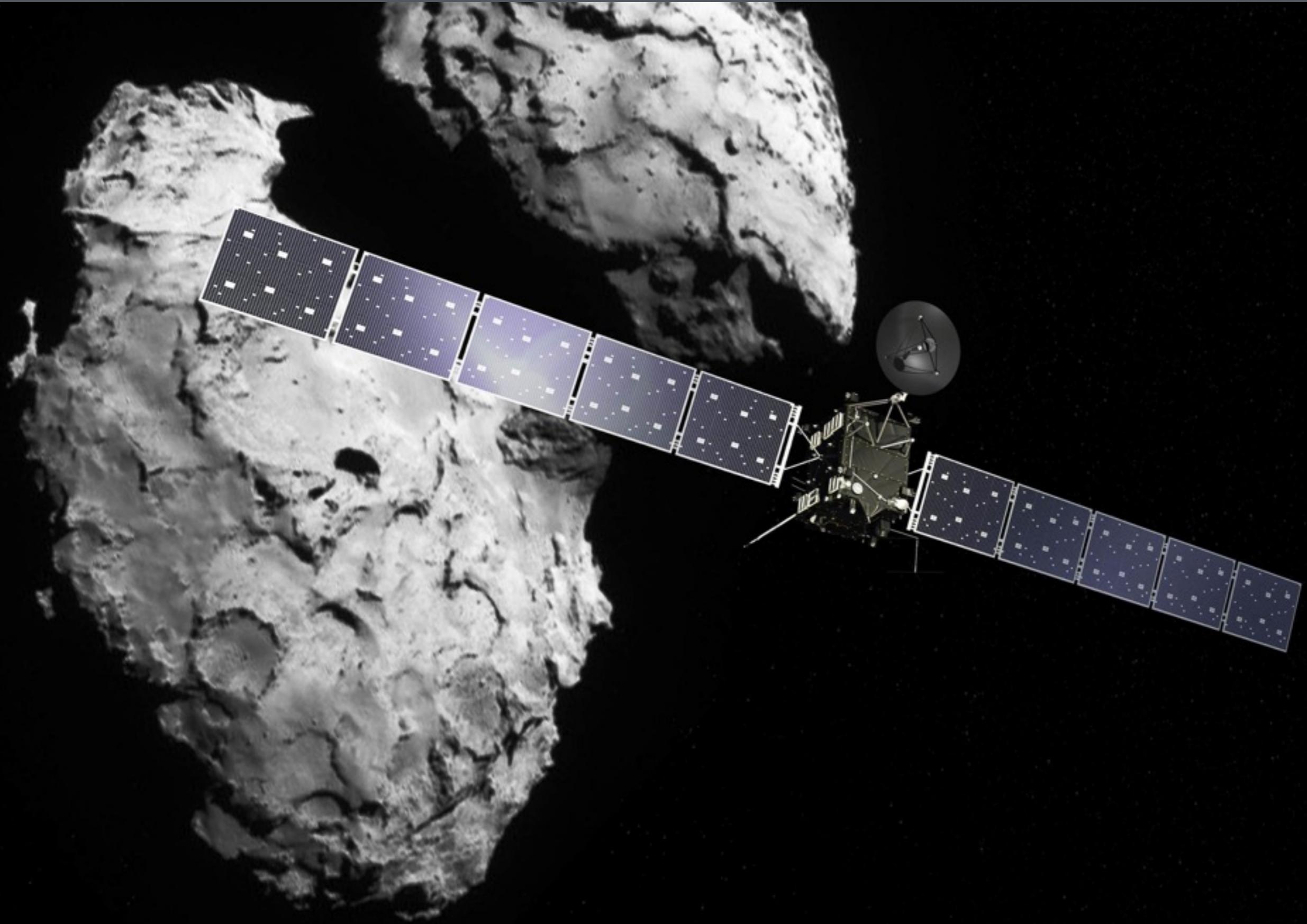
In school/university, you learn the basic fundamental laws. Examples are easy. You do them with pen and paper. Real life is more complicated.

# How you learn physics in school/university



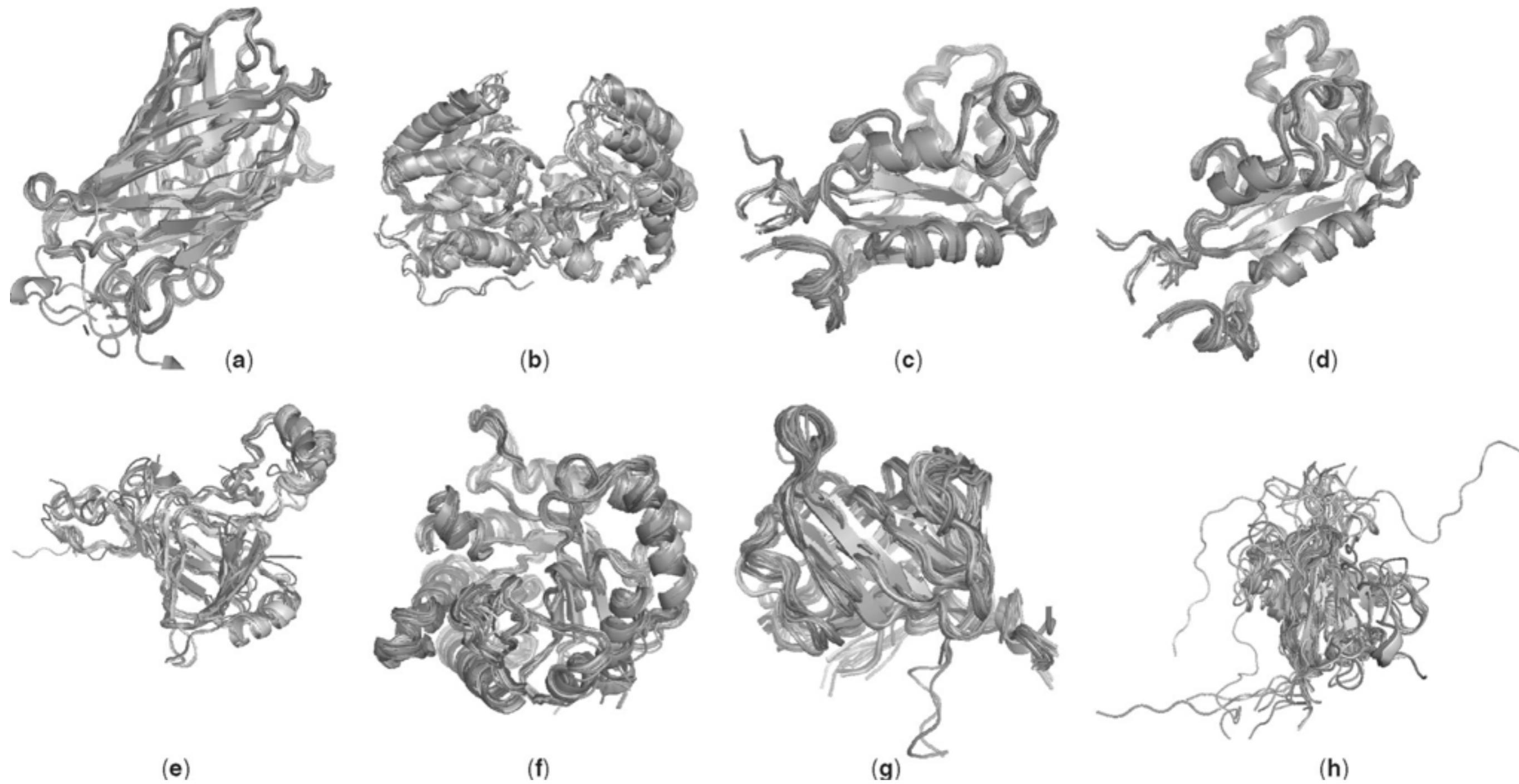
$$F_g = \frac{GMm}{d^2}$$

If you do science, it's more complicated





# Chemistry



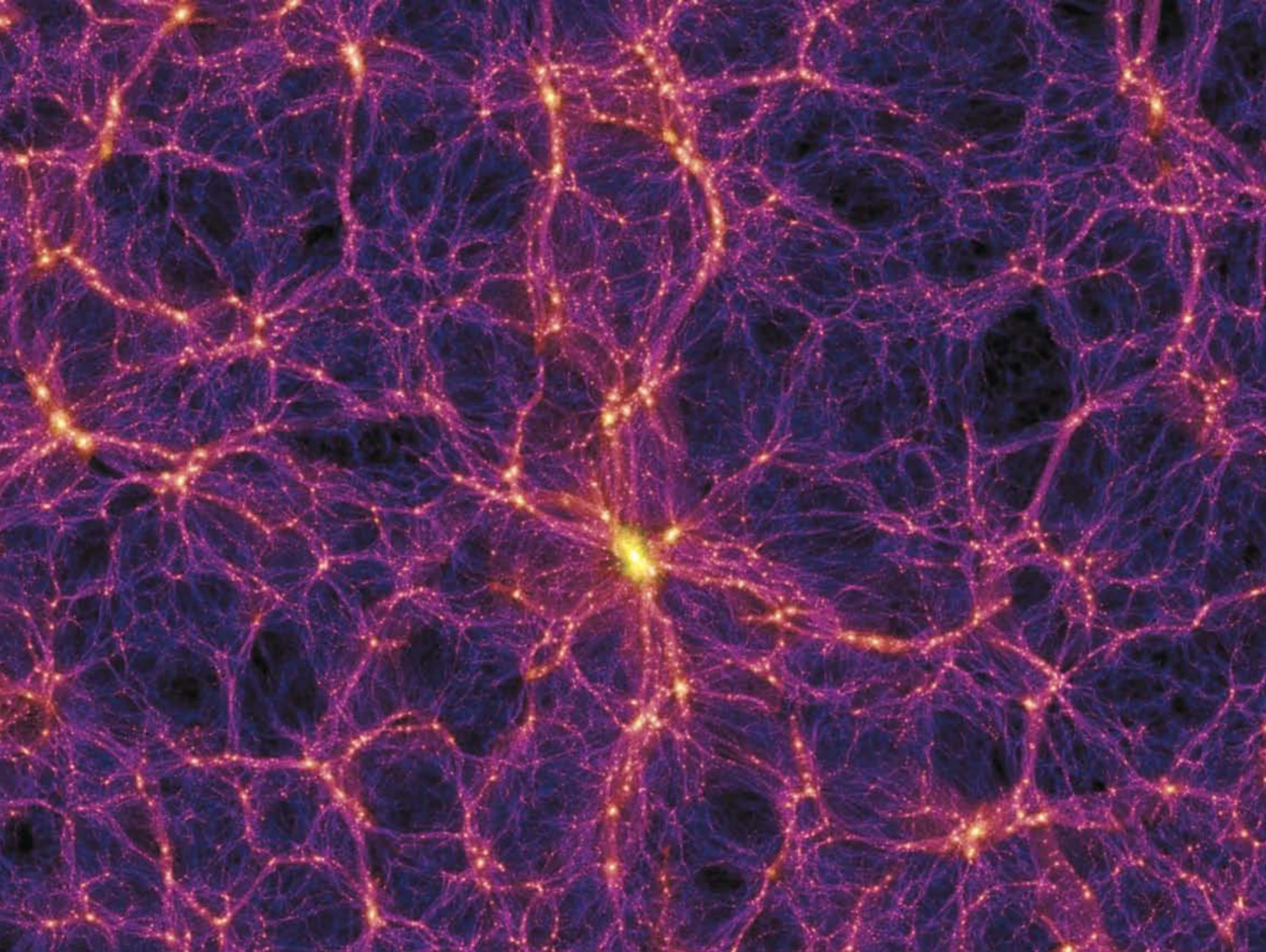
# Why do we need scientific computing?

## 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.

## 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.



# Why do we need scientific computing?

## Complexity

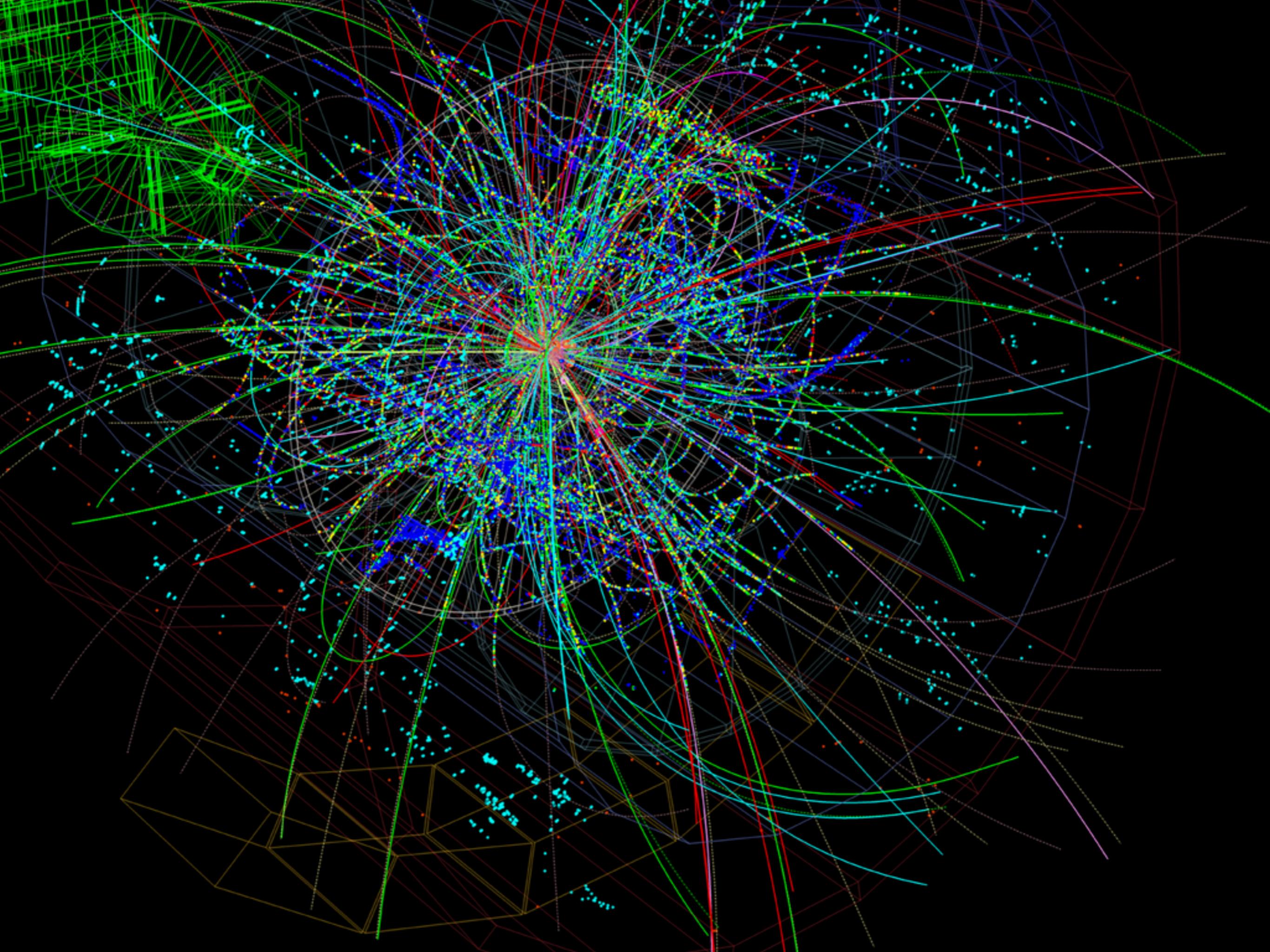
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## Simulations

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.

## 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**

## 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.

—> **You should have some basics programming skills, but you'll learn how to apply them in PSCB57**

# Skills, tools needed for scientific computing

## Mathematics

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

## Discretization

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

## Programming

Python, 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 phones, no food

# Assignments

Total of 6 assignments, difficulty varies

**Submit source code online**

<http://rein.utsc.utoronto.ca/submit>

username: pscb57, password: 2016

I highly recommend to test your submission

Submission is either right or wrong

You have to pass quiz in next tutorial

# Assignments

## Introduction to Scientific Computing, PSCB57, Fall 2016

### Assignment 1

#### Python and Fibonacci numbers

- The deadline for the assignment is Friday, September 9th, 5pm.
- You must submit the assignment electronically at <http://rein.utsc.utoronto.ca/submit/>. On the same website, you can run an automated check of your program before submitting it.
- The username is `pscb57`, the password is `2016`.
- You must be present at the tutorial in the following week to take a quiz. If you do not show up or fail to pass the quiz, your assignment will be marked as 0% even if it was correct.
- Plagiarism is taken very seriously. However, you are not expected to work in solitude and are encouraged to talk to your classmates. But keep in mind that if you submit an assignment, you have to fully understand it in order to pass the quiz.

Write a program to calculate the first 10 odd Fibonacci numbers. The output of your program should be:

```
1  
1  
3  
5  
13  
21  
55  
89  
233  
377
```

In addition, the program also needs to satisfy the following criteria:

- The program has to be written in python3.
- You may not use of any packages or libraries, i.e. do not use the `import` statement.
- The entire program has to be 50 lines of code or less (including comments).
- The runtime of your program has to be 1 second or less.
- The program may not contain hard coded Fibonacci numbers other than the first two: 0 and 1. The program needs to calculate the Fibonacci numbers in a loop or with a recursive function. Your program should be easy to modify. As an example, try to output the first 10 odd numbers.

# Quiz example

## Submitted code

```
1     i = 1
2     a = 0
3     b = 1
4     while i < 10:
5         if (b % 2 != 0):
6             print(b)
7         tmp = b
8         b = tmp
```

## Code with bugs

```
1     i = 0
2     a = 0
3     b = 1
4     while i > 1000:
5         if (b % 2 != 2):
6             print(b)
7         tmp = b
8         a = tmp
```

# Quiz example

Name	Class	Quiz
Name Not Found	PSCB57 Fall 2016	Quiz1

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	A	B	C	D	E	A	B	C	D	E	A	B	C	D	E	A	B	C	D	E
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Do not fold or bend sheet  
or erase mistakes completely

# Software

You have to be able to run python3 code.

1. Use your own computer. Linux or MacOS. For Windows, need to install anaconda or virtual machine. Setting this up, is up to you.
2. Use UTSC computer labs (BV).
3. Use computers in physics labs (SW).
4. Get remote access to a linux machine.

# Remote access

- If you want to make use of this, come to my office to setup an account.
- On any computer, download an ssh client such as putty or MobaXterm.
- You can login to `rein001.utsc.utoronto.ca` from anywhere.
- You'll need to get comfortable working with linux!

# Python

# Why python?

- Becoming the industry standard 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 strongly-typed

```
a = 9  
b = "9"  
c = a+b      // exception
```

# 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
- At the end of this course, we'll use another language, julia, which is “*as fast as C*”

# 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.

# Number representations

