# Computational Mathematics
# Lecture 1

Patrick E. Farrell

University of Oxford

Section 1

# Computational mathematics by example

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$$d(n) = 0.4 + 0.3 \times 2^n, \quad n = -\infty, 0, 1, \ldots.$$

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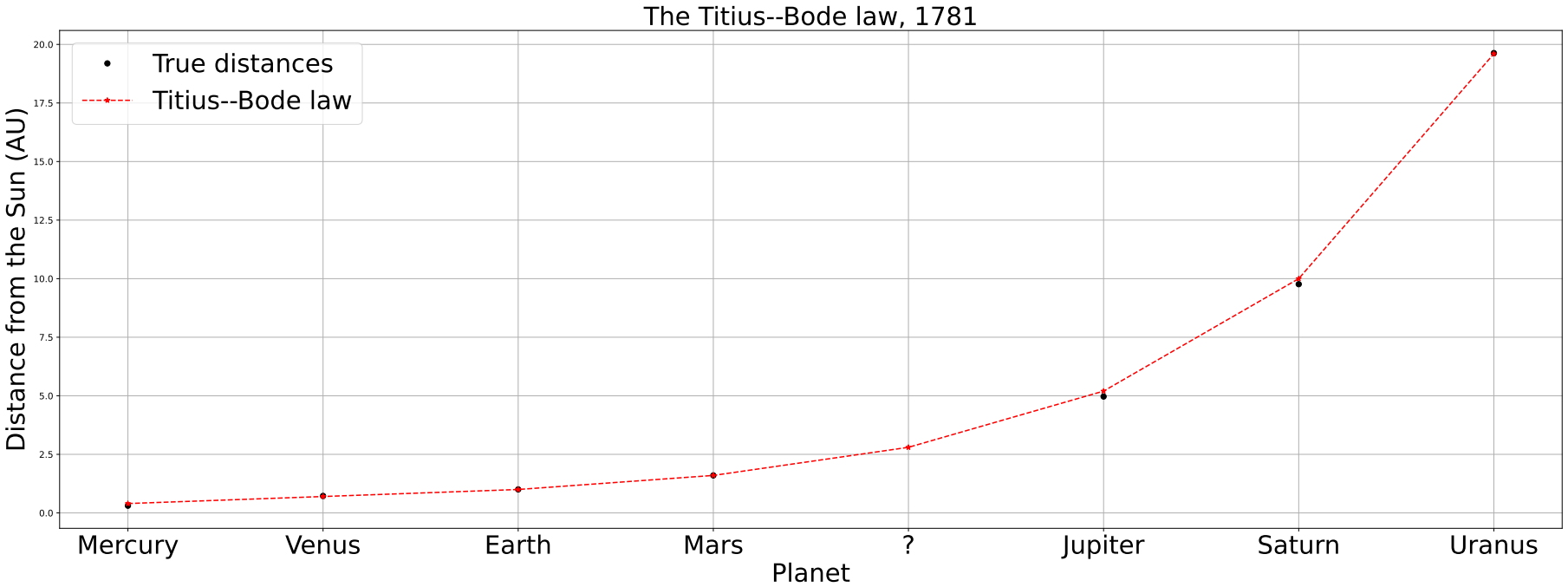

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On 1 January 1801, Giuseppe Piazzi discovered Ceres, almost exactly where the Titius–Bode law predicted!

But he could only observe it for 41 days before it was lost behind the Sun—not long enough to compute its orbit. How could it be found again?

Giuseppe Piazzi, 1746–1826

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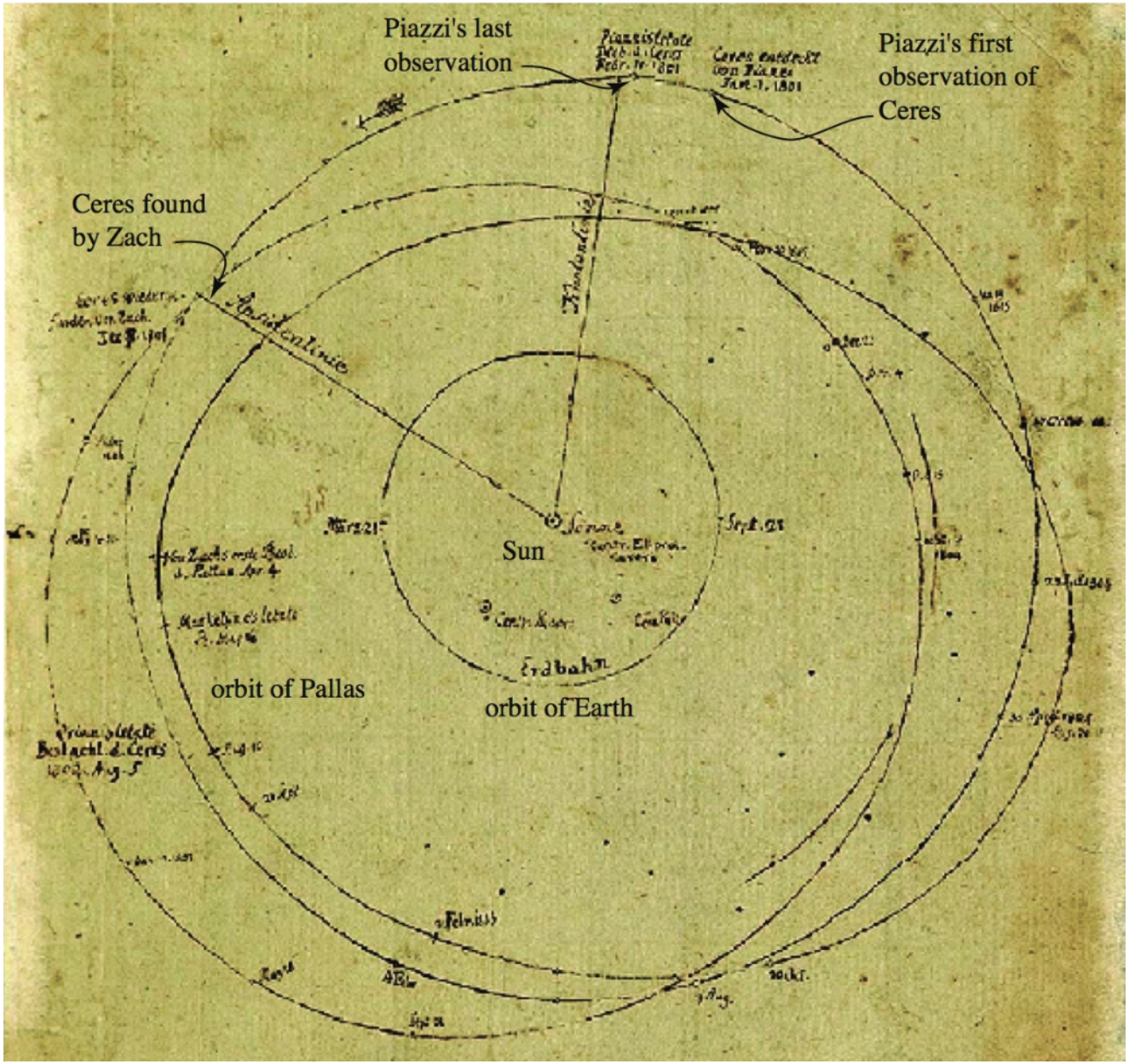
Gauss knew that orbits are approximately ellipses with the sun at one focus, which left him with six parameters to estimate from Piazzi's 22 observations.

Gauss calculated for weeks on end; he published his prediction for Ceres' location in September 1801. On December 7, astronomers found Ceres again, almost exactly where he predicted.




Annotated sketch from Gauss' papers. Courtesy Georg-August-Universität Göttingen.

It is possible to find two squares that sum to a square:

$$3^2 + 4^2 = 5^2,$$

and three cubes that sum to a cube:

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But Euler could not find natural solutions to

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So, in 1769, Euler conjectured that

$$\exists\, k > 1, n > 1, a_1, \ldots, a_n, b \in \mathbb{N}_+ : a_1^k + a_2^k + \cdots a_n^k = b^k \implies k \leq n.$$

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In 1966, Leon J. Lander and Thomas R. Parkin discovered a counterexample:

## COUNTEREXAMPLE TO EULER'S CONJECTURE ON SUMS OF LIKE POWERS

BY L. J. LANDER AND T. R. PARKIN

Communicated by J. D. Swift, June 27, 1966

A direct search on the CDC 6600 yielded

$$27^5 + 84^5 + 110^5 + 133^5 = 144^5$$

as the smallest instance in which four fifth powers sum to a fifth power. This is a counterexample to a conjecture by Euler [1] that at least $n$ $n$th powers are required to sum to an $n$th power, $n > 2$.

### Reference

1. L. E. Dickson, *History of the theory of numbers*, Vol. 2, Chelsea, New York, 1952, p. 648.

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This is equivalent to colouring a *graph*: each region is a vertex, and adjacent regions are connected with an edge.

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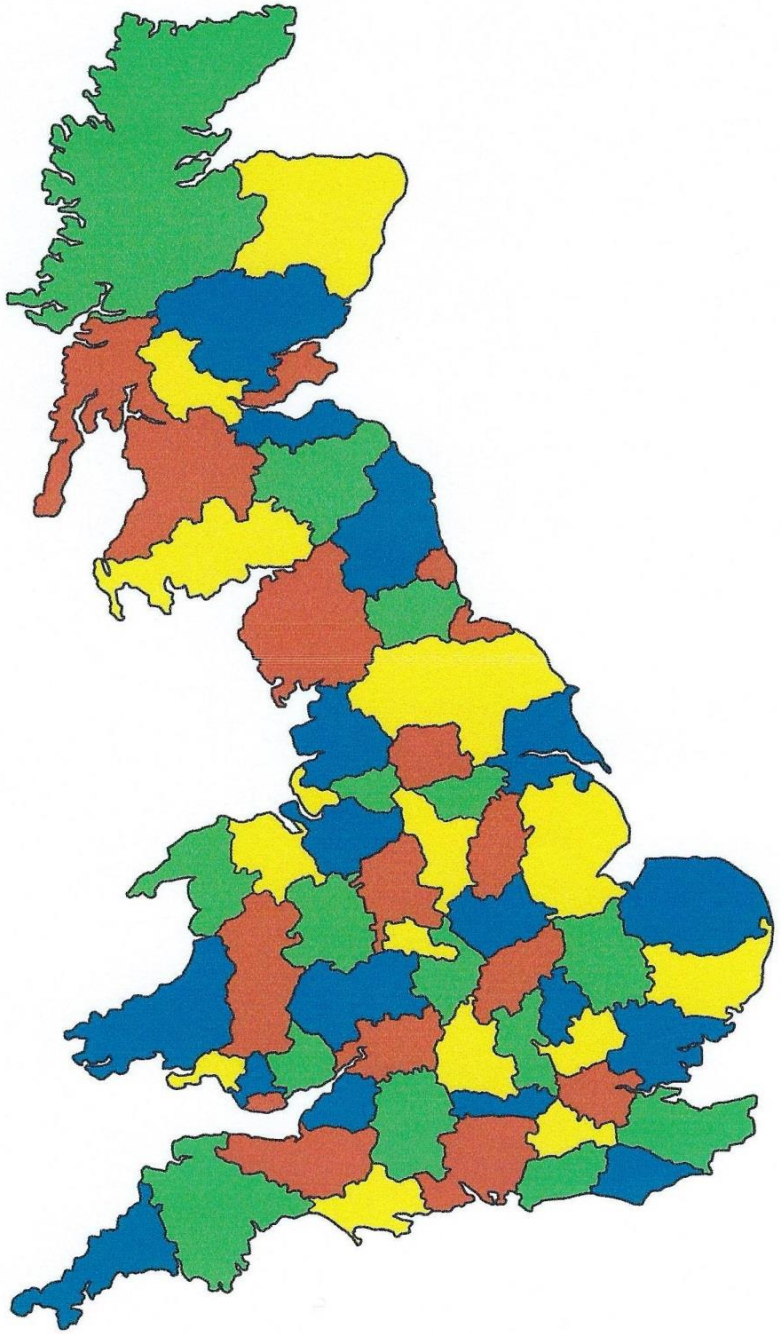

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While the proof was wrong, the basic strategy was right.

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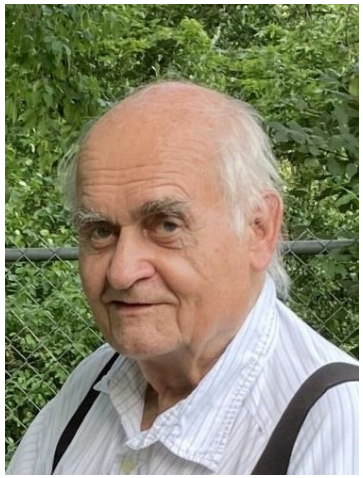

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With a computer, they found an unavoidable set with 1834 cases, and programmed it to mechanically check that in each case the graph can be coloured with four colours.

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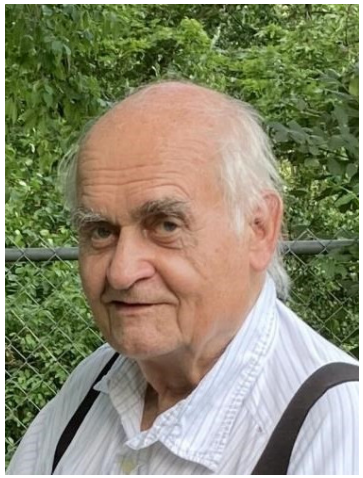

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Since then, many theorems have been proven with computer-assisted proofs, among them

- Kepler's conjecture on packing cannonballs;
- Keller's conjecture on tiling Euclidean space;
- Feigenbaum's conjecture in dynamical systems.

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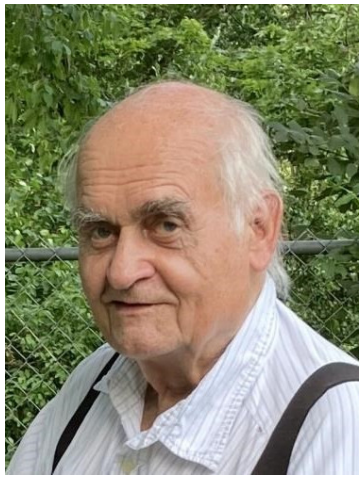

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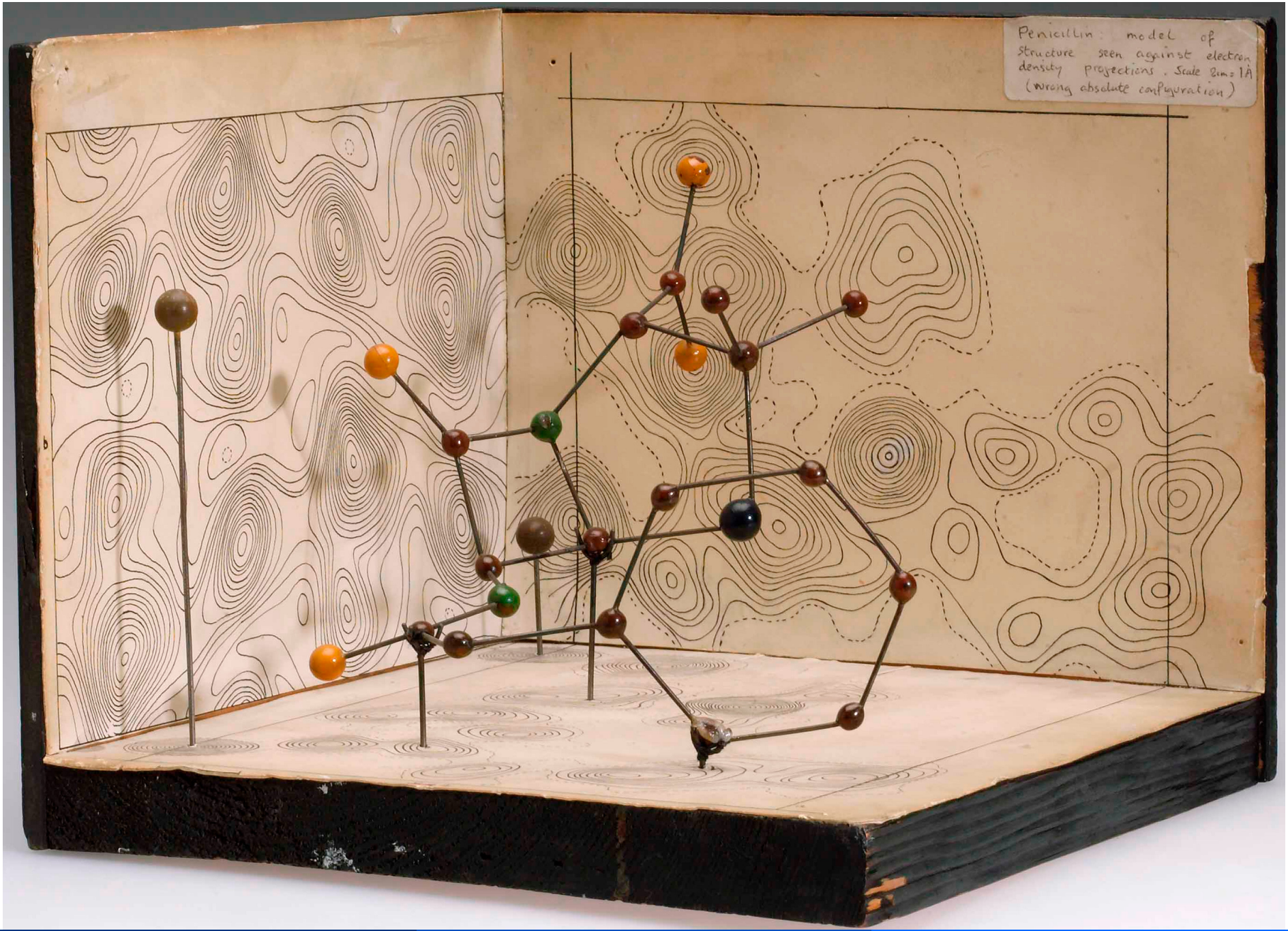
The calculations involved least squares, Fourier analysis, and extensive use of group theory.


Penicillin: model of
structure seen against electron
density projections. Scale 2in = 1Å
(wrong absolute configuration)

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In 1964 she won the Nobel Prize in Chemistry for her identification of penicillin and vitamin $B_{12}$.

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These problems might be in pure mathematics (Euler's Conjecture in number theory, the Four-Colour Theorem in graph theory), or in applied mathematics (Gauss' discovery of the orbit of Ceres, Hodgkin's work in crystallography).

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Computational mathematics is an ancient subject; it did not begin with the invention of computers. Instead, *computers were invented to speed up computational mathematics!*

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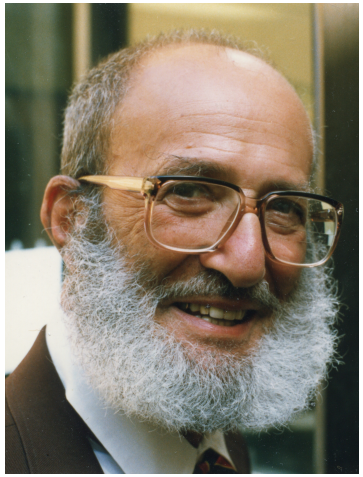
> *When you try to prove a theorem, you don't just list the hypotheses, and then start to reason. What you do is trial and error, experimentation, guesswork. You want to find out what the facts are.*



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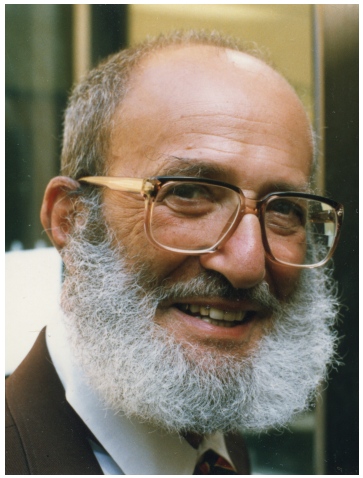

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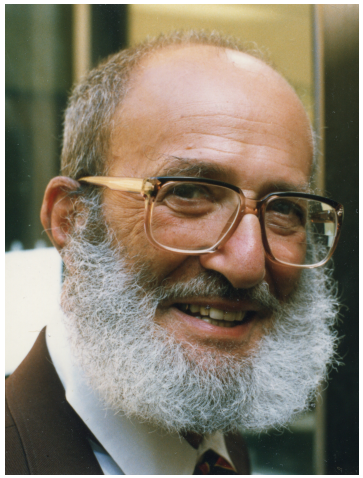

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As G. H. Hardy wrote,

> *The theory of numbers, more than any other branch of mathematics, began by being an experimental science. Its most famous theorems have all been conjectured, sometimes a hundred years or more before they were proved; and they have been suggested by the evidence of a mass of computations.*

Godfrey Hardy, 1877–1947

Section 2

# Practicalities

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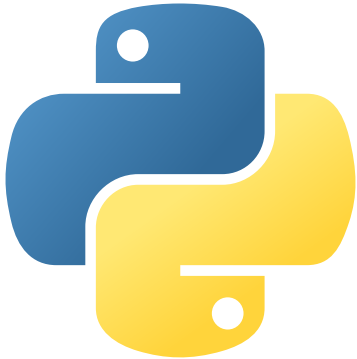
On a pragmatic point, a very large fraction of Oxford mathematics graduates will pursue careers where programming is useful, if not essential. These include

- mathematical research;
- scientific research;
- quantitative finance;
- teaching;
- data science;
- management consulting.

In this course, we will learn the Python programming language.



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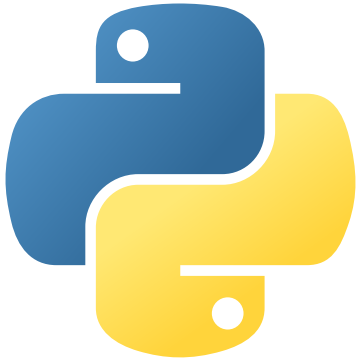

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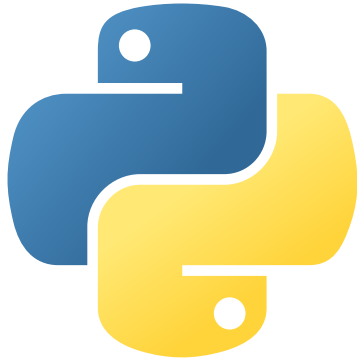

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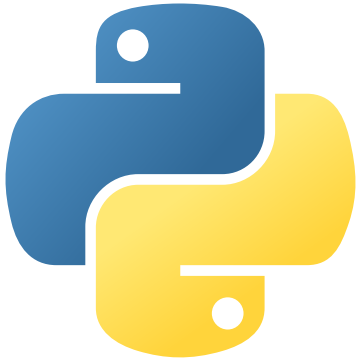

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Guido van Rossum, 1956–

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|---|---|---|---|
| 1–2 MT | 1–3 | - | - |
| 3–4 MT | 4–5 | - | 1 |
| 5–6 MT | 7 | 8 | 2 |
| 7–8 MT | 10 | - | 3 |
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There are four two-hour demonstration sessions for this course; three this term, and one next term. In demonstration session $n$ you start problem sheet $n$, and return it for marking in demonstration session $n + 1$.

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This term's work forms the basis for your projects in Hilary term. Three projects will be announced; you choose two of them. The projects are done in the same manner as the problem sheets for this term, but with more emphasis on interweaving coding, mathematics, and discussion.

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(Optionally) bring your laptops along to the next lecture to follow along with installation.

$\rightarrow$ the Lander–Parkin counterexample

# Computational Mathematics
# Lecture 2

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University of Oxford

## How to submit problem sheets

## A brief tour of the course

- Week 3–4 MT
- Week 5–6 MT
- Week 7–8 MT
- Week 1–2 HT

## Software installation

Section 1

# How to submit problem sheets

$\rightarrow$ using `publish.py`

Section 2

# A brief tour of the course

Week 3–4 MT teaches

- arithmetic,
- conditionals,
- iteration.

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*If $f : [a, b] \to \mathbb{R}$ is continuous with $f(a)f(b) < 0$, then there exists $x^\star \in (a, b)$ with $f(x^\star) = 0$.*

The statement $f(a)f(b) < 0$ is just a fancy way of saying $f(a)$ and $f(b)$ have opposite signs.

Bernhard Bolzano, 1781–1848

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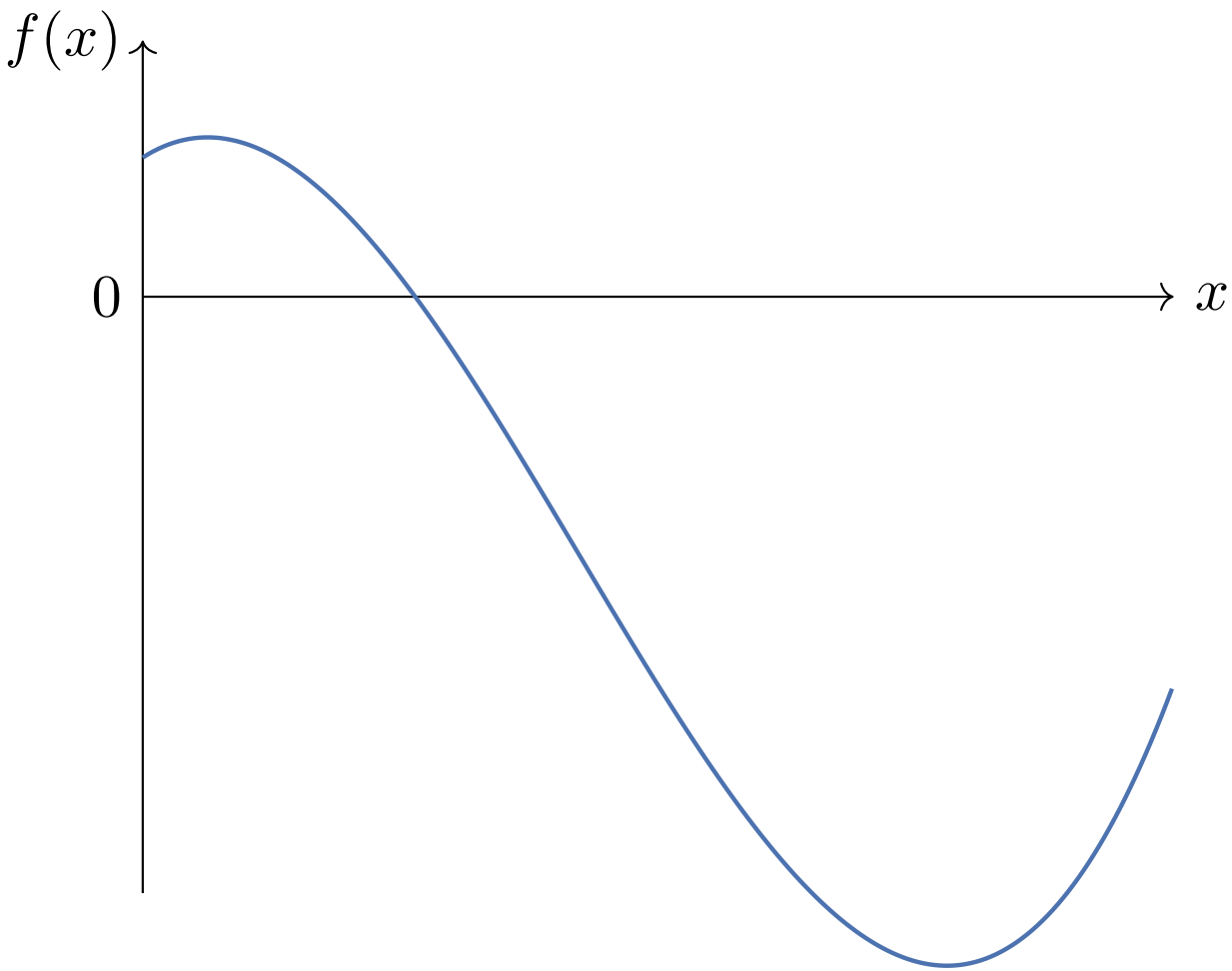
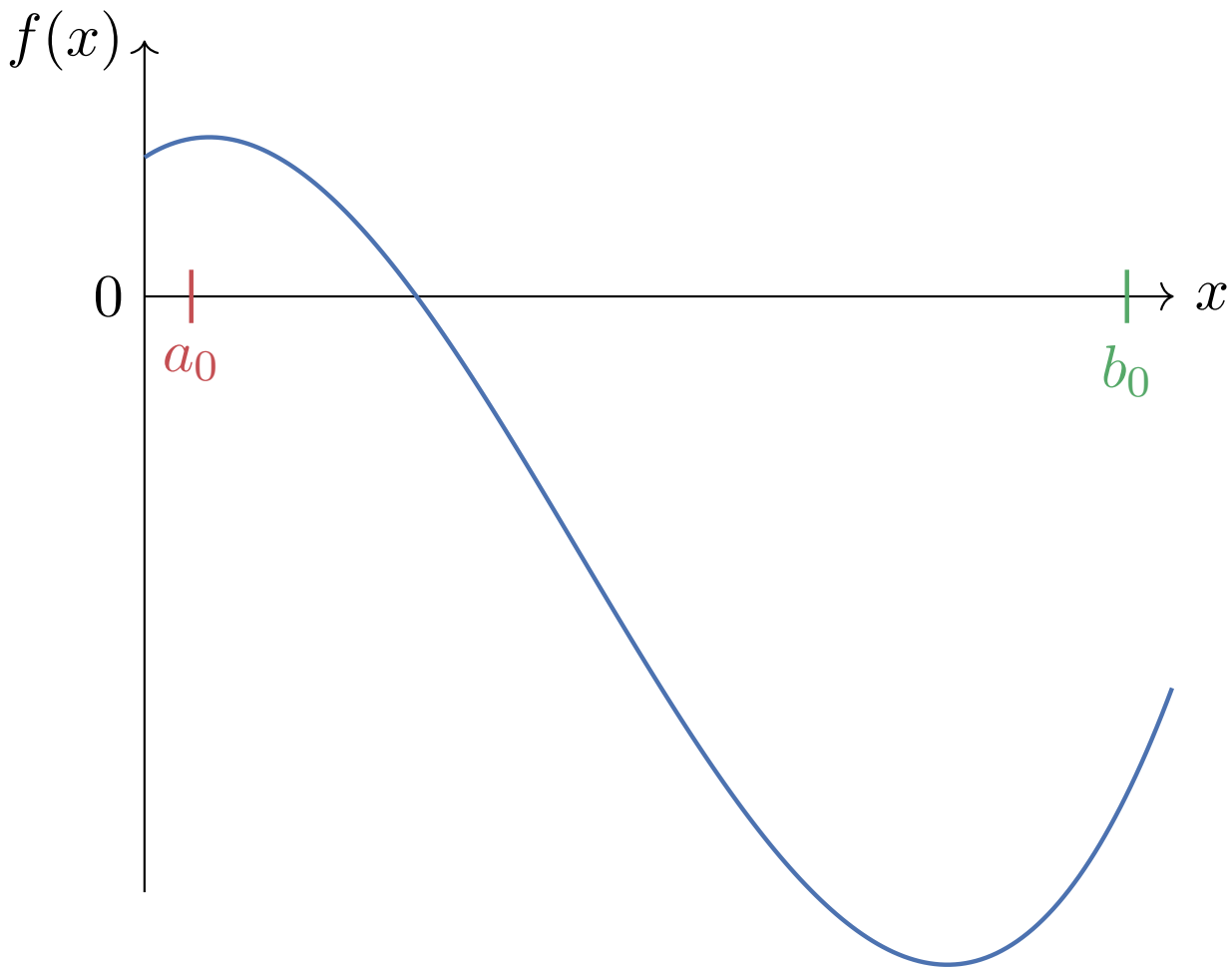
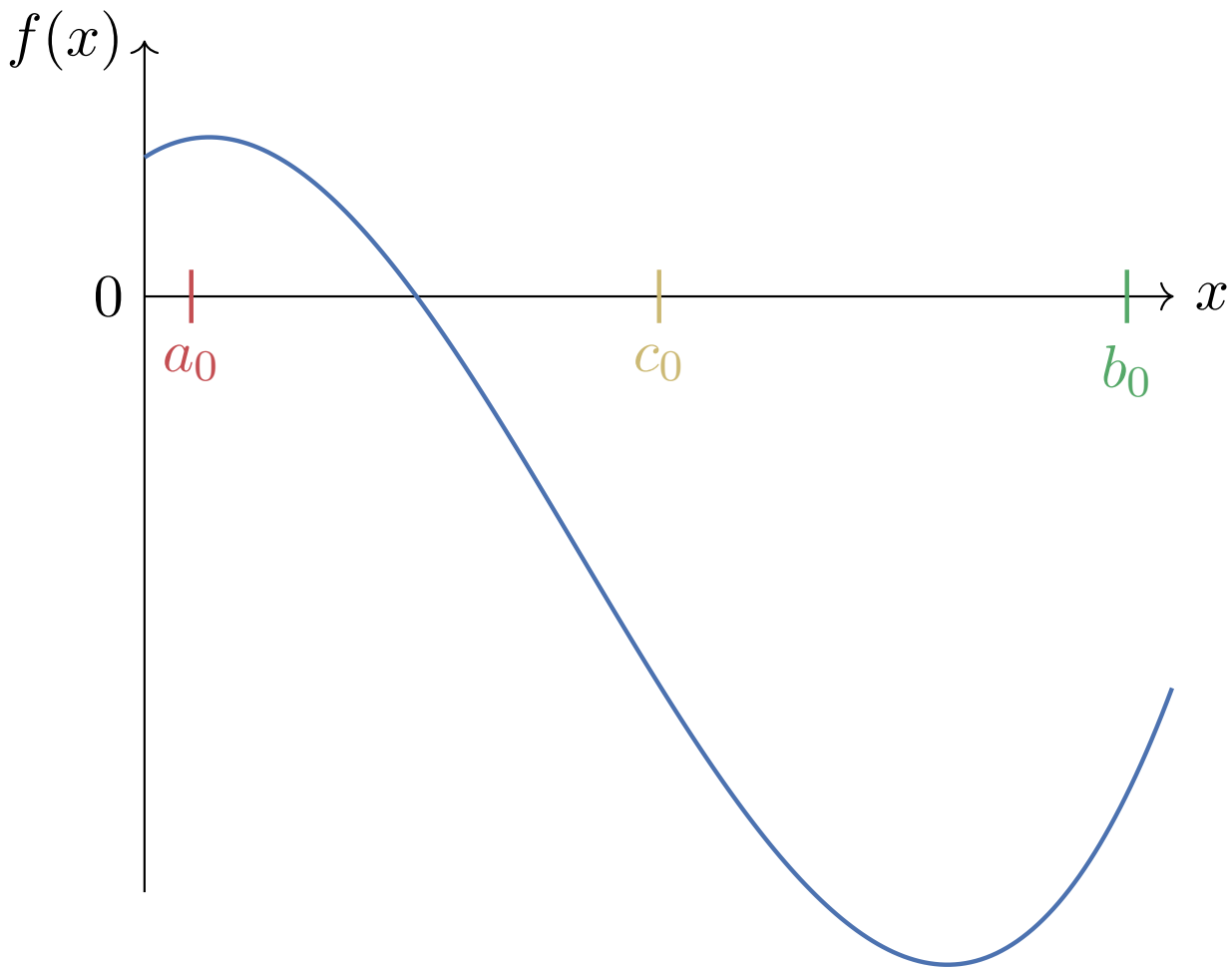
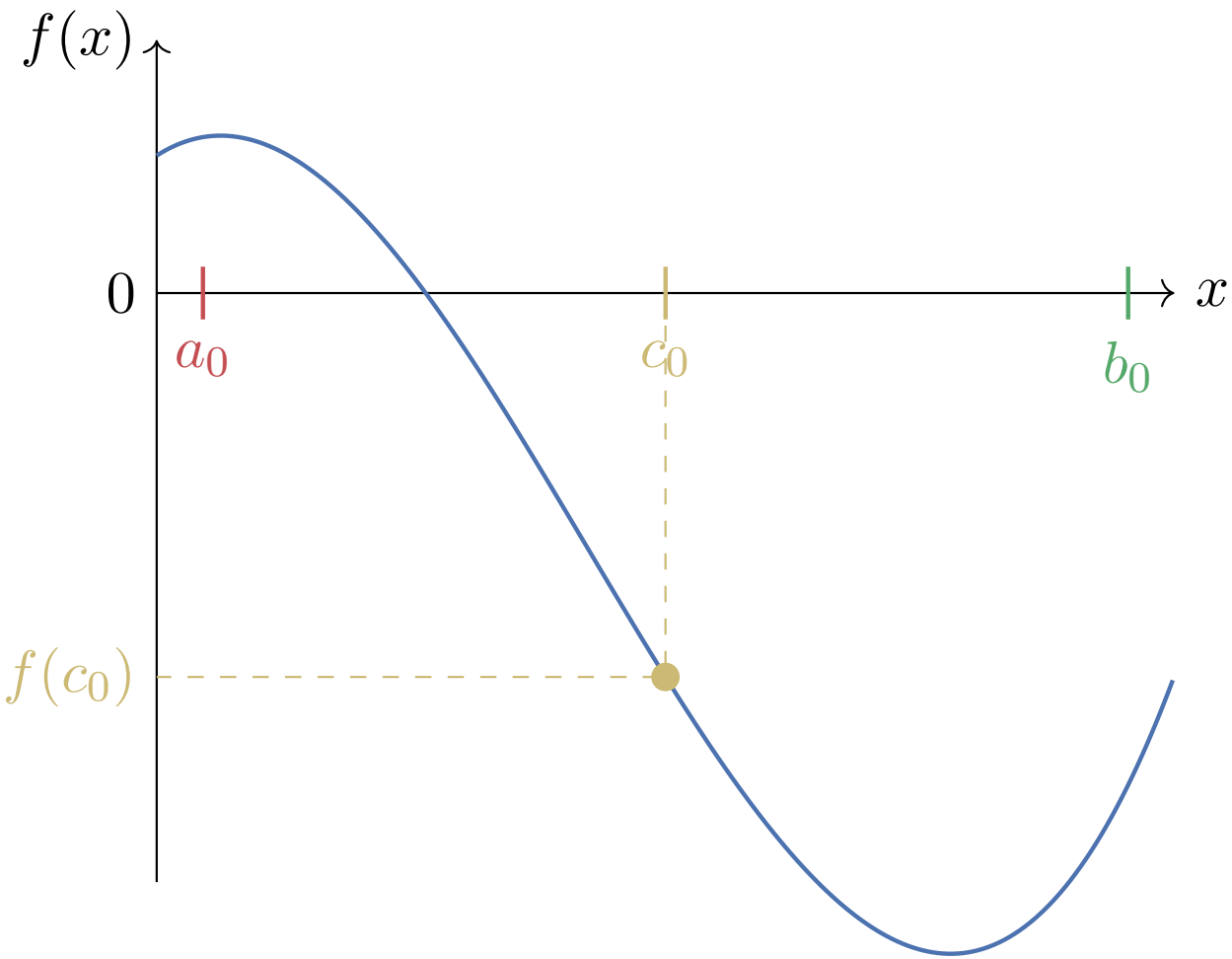
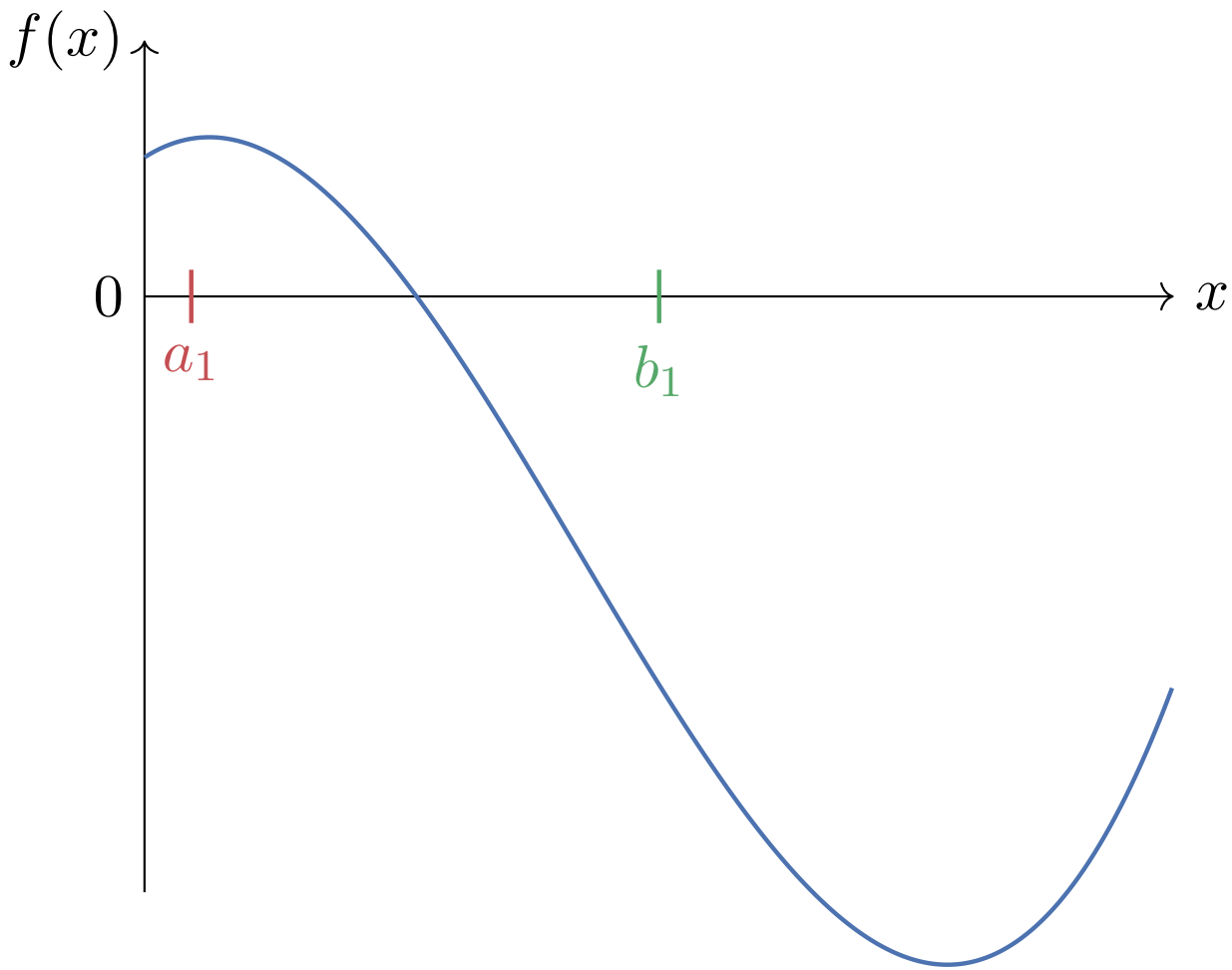
3. $f(c)$ has the same sign as $f(b)$, so there exists a root in $(a, c)$.

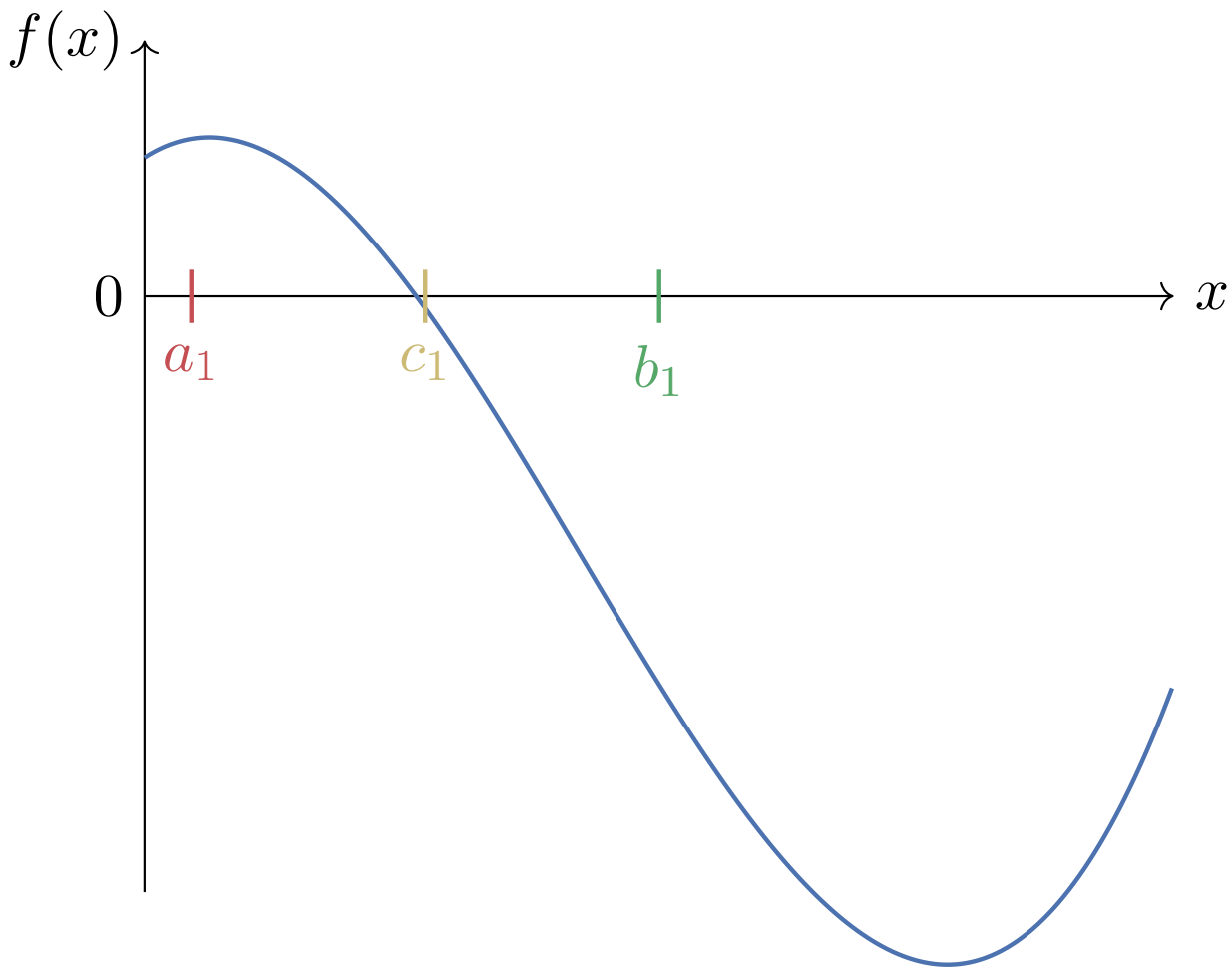

$f(x)$
0
$x$

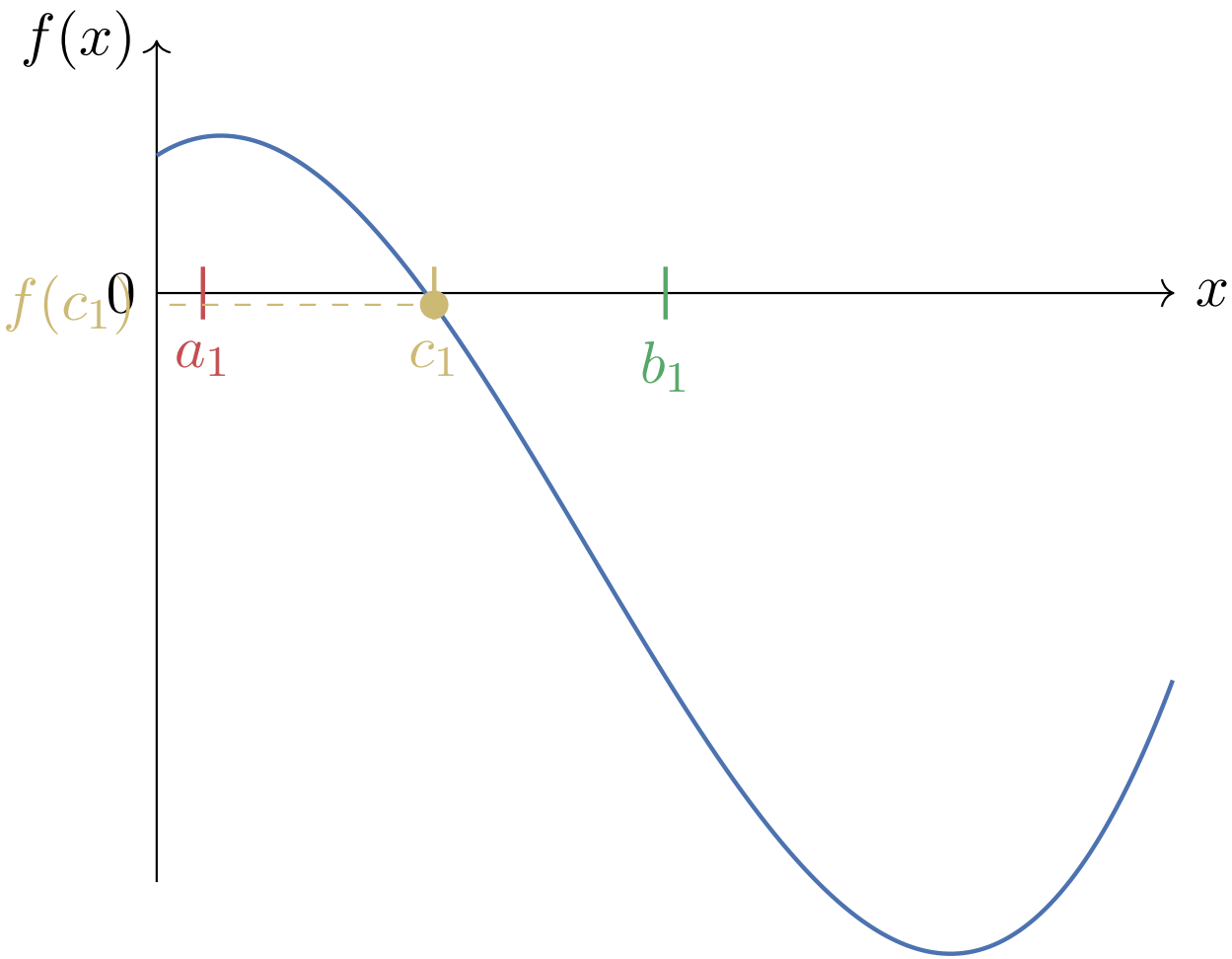

$f(x)$
0
$a_0$
$b_0$
$x$

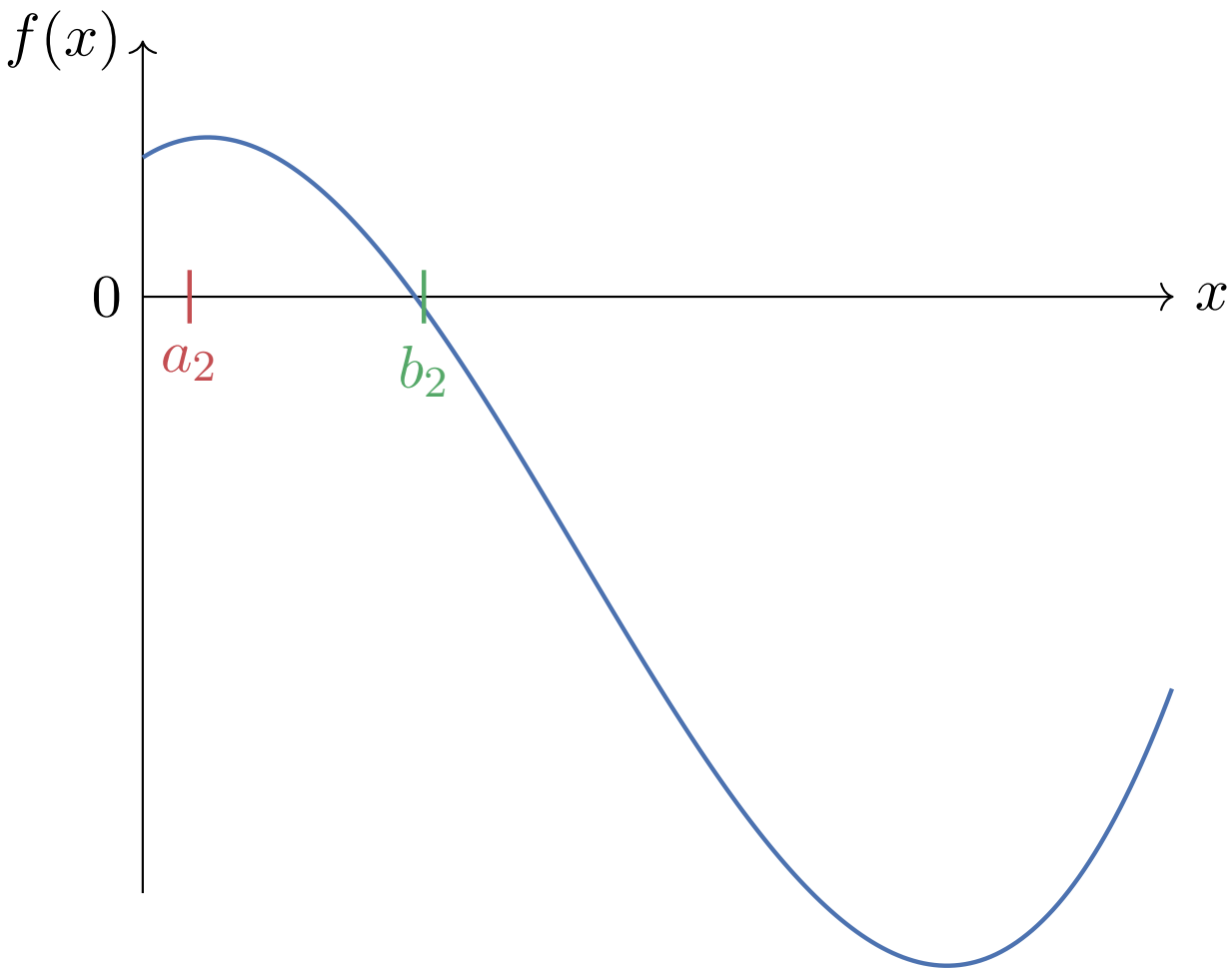

$f(x)$
0
$x$
$a_0$
$c_0$
$b_0$

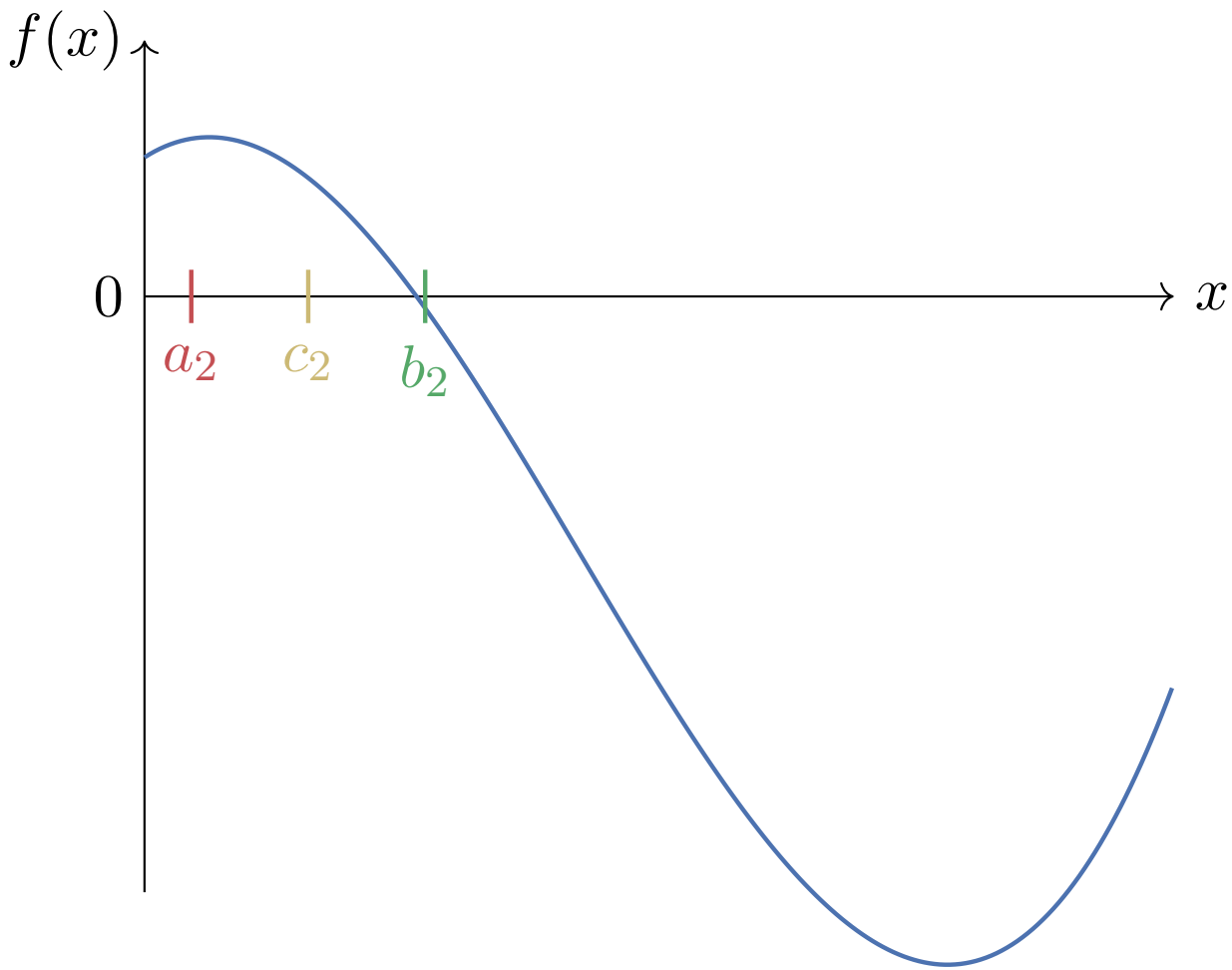

$f(x)$
$0$
$x$
$a_0$
$c_0$
$b_0$
$f(c_0)$

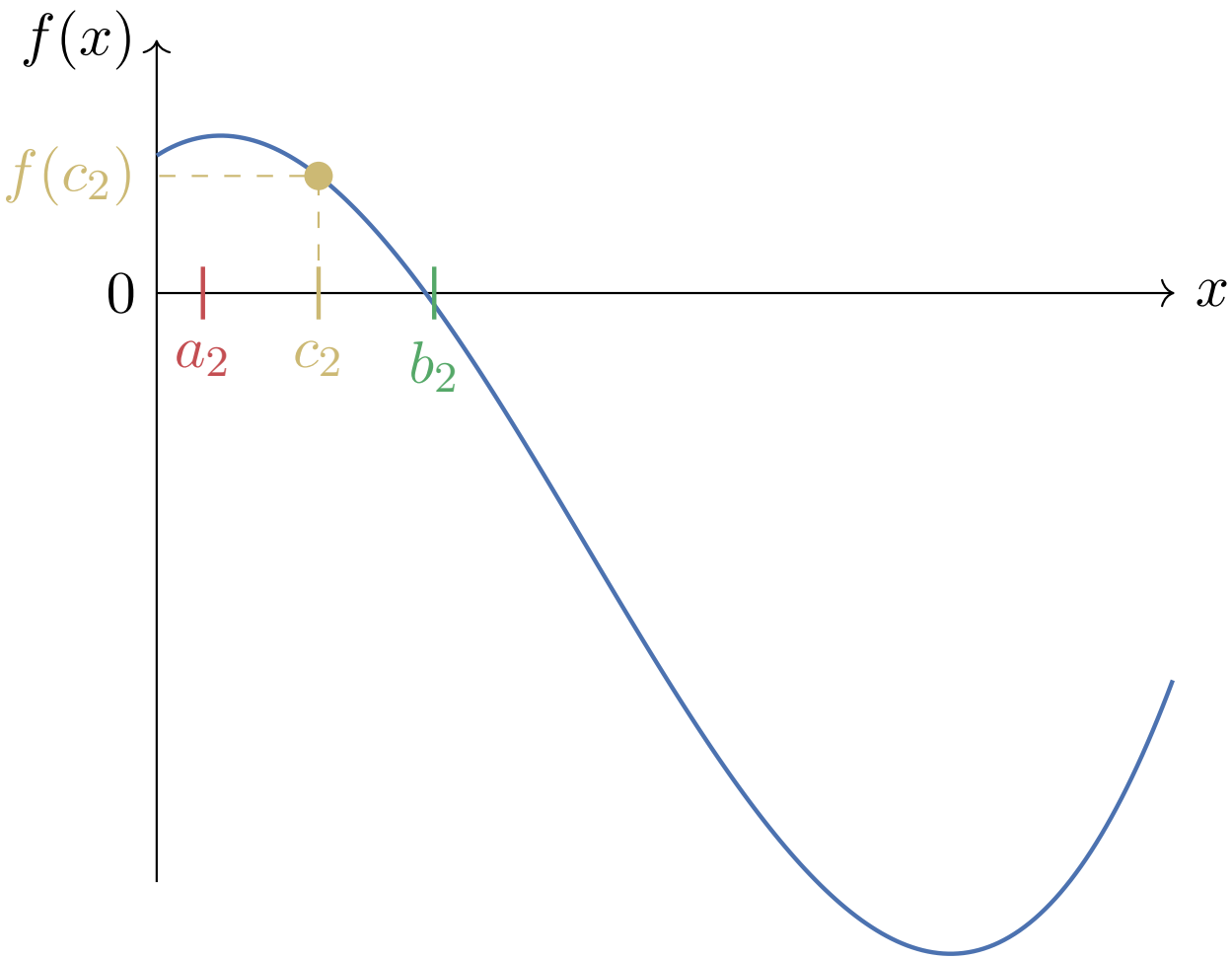

$f(x)$
0
$x$
$a_1$
$b_1$

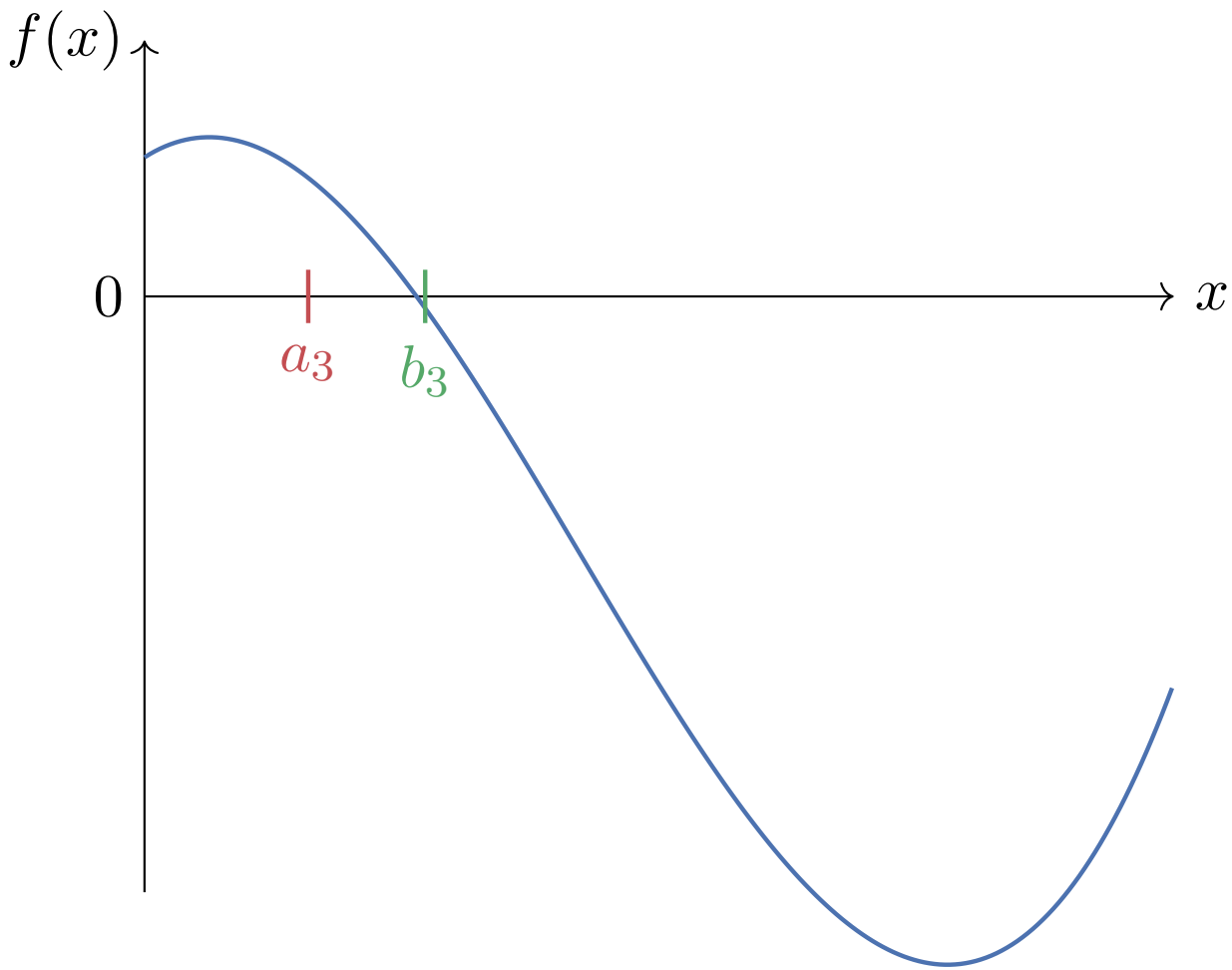

$f(x)$
0
$x$
$a_1$
$c_1$
$b_1$

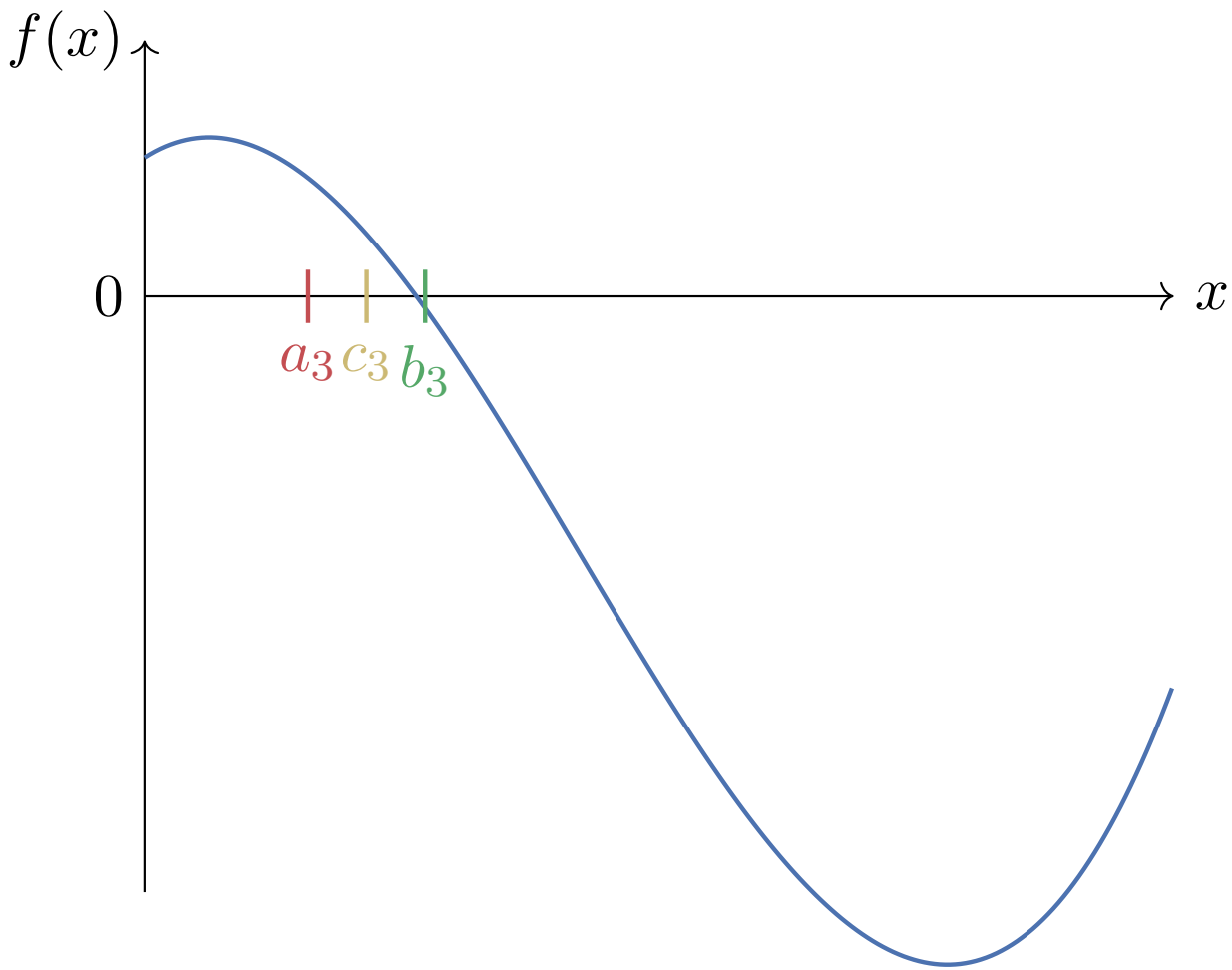

$f(x)$
$f(c_1)0$
$x$
$a_1$
$c_1$
$b_1$

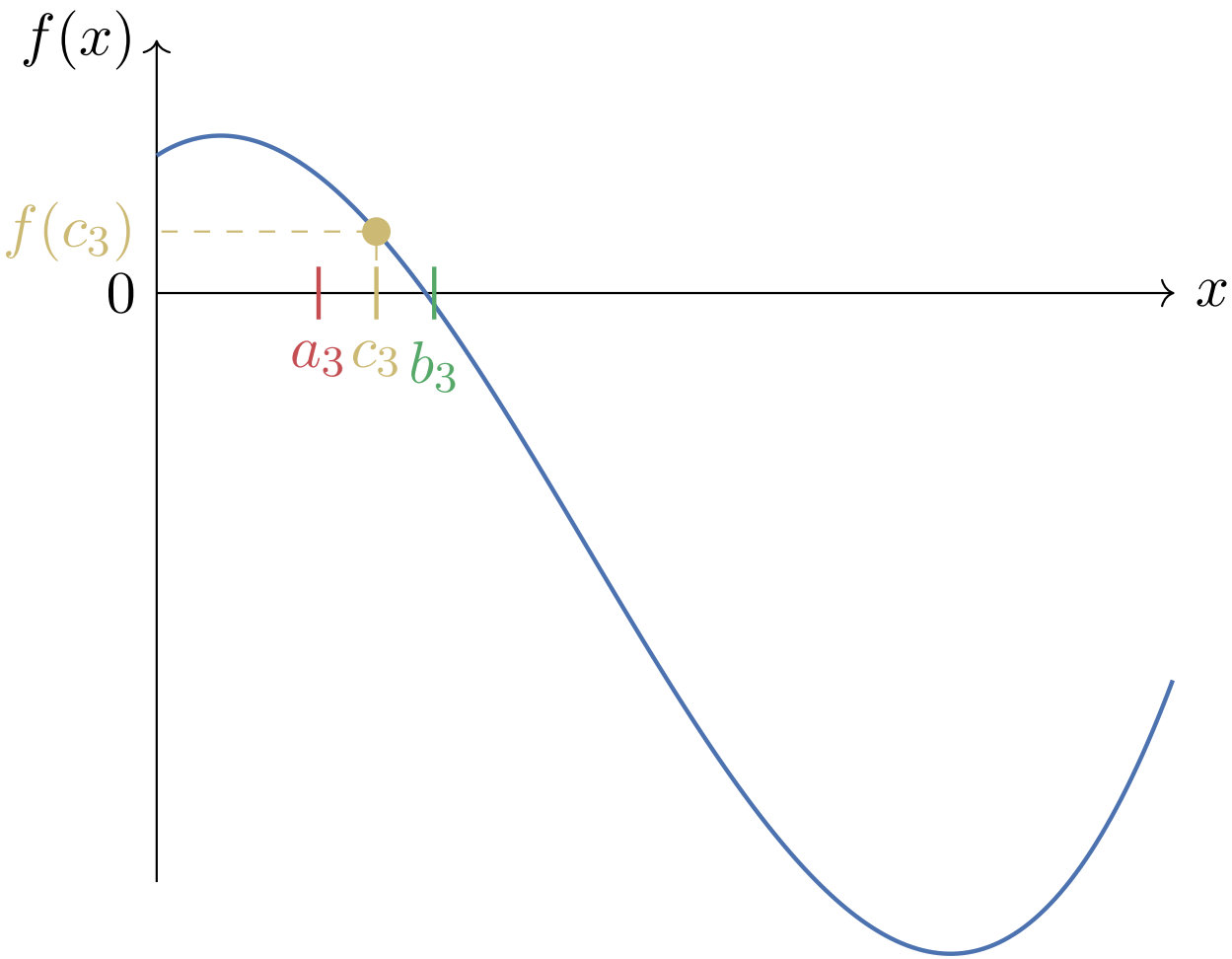

$f(x)$
0
$x$
$a_2$
$b_2$

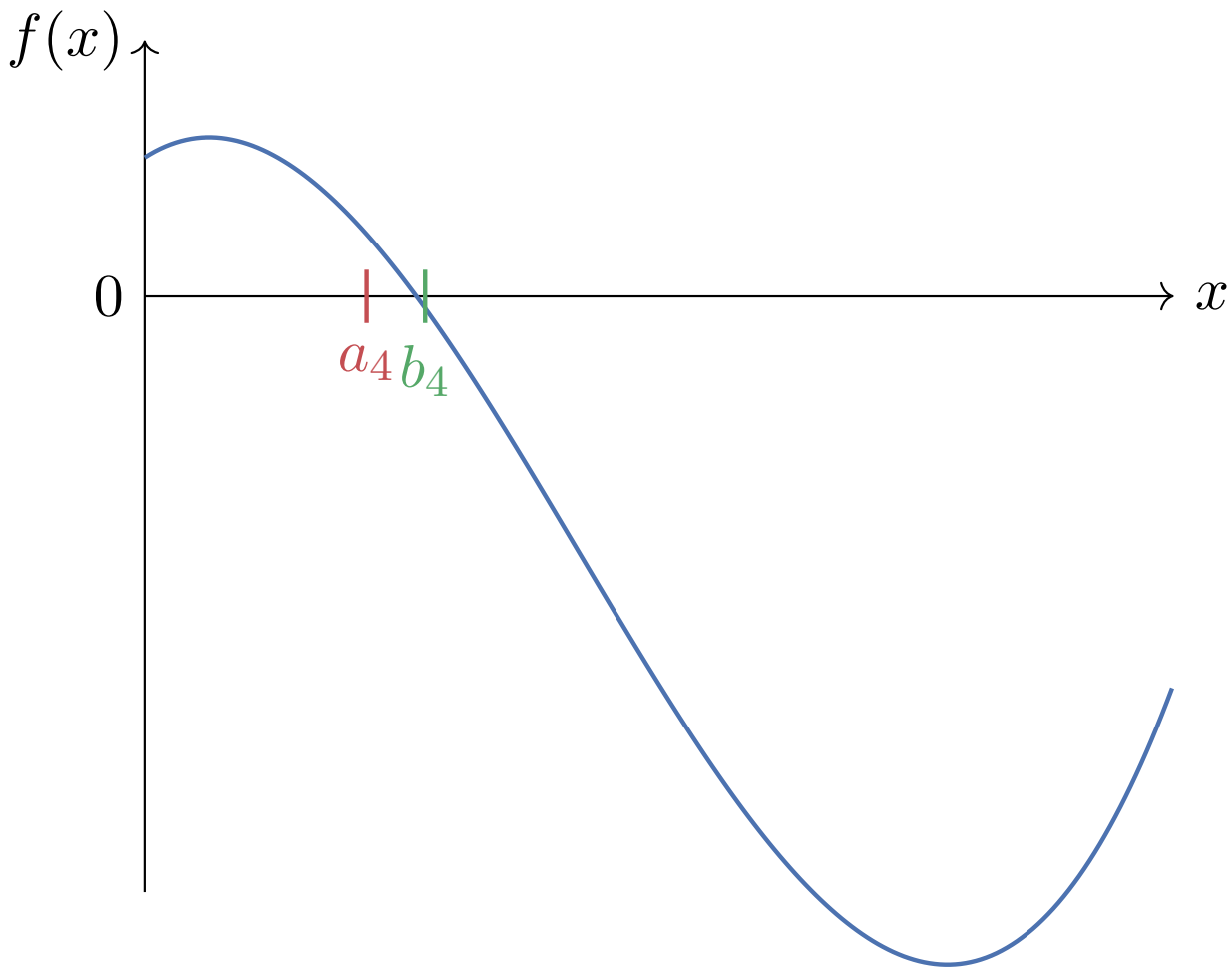

$f(x)$
0
$x$
$a_2$
$c_2$
$b_2$


$f(x)$
$f(c_2)$
0
$a_2$
$c_2$
$b_2$
$x$


$f(x)$
0
$x$
$a_3$
$b_3$


$f(x)$
0
$x$
$a_3$
$c_3$
$b_3$


$f(x)$
$f(c_3)$
0
$x$
$a_3$ $c_3$ $b_3$


$f(x)$
0
$x$
$a_4$
$b_4$

$\rightarrow$ `bisection.py`

How can we use this to compute an approximation to $\pi$?

Week 5–6 MT teaches

- lists, tuples
- dictionaries, sets,
- functions,
- plotting.

Week 5–6 MT ends with a naïve code for *primality testing*, checking whether a given integer is prime or not.

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→ `isprime.py`

Can we make `isprime(9999991111111)` faster?

Week 7–8 MT introduces *symbolic computing*, the use of computers to automate the kind of mathematical manipulations you do on paper.

This includes expanding and simplifying expressions, differentiating and integrating functions, calculating limits, and solving equations.

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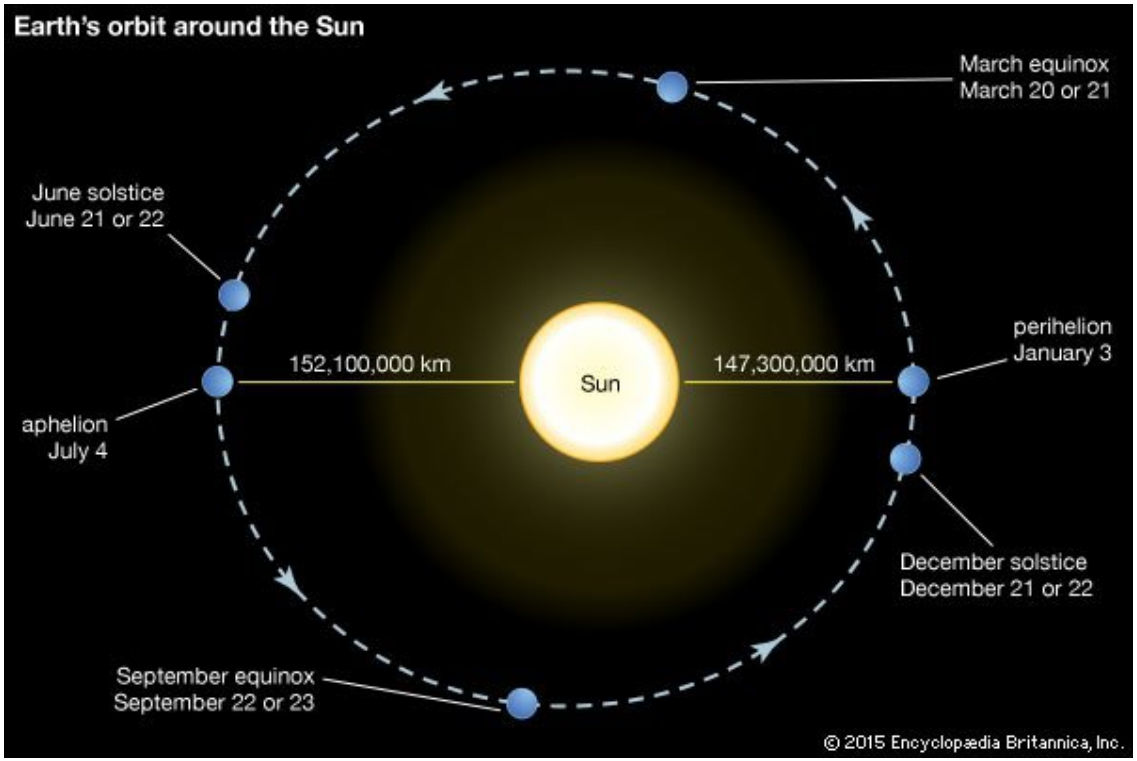
In 1843, describing Charles Babbage's Analytical Engine, Ada Lovelace wrote

> *Many persons who are not conversant with mathematical studies imagine that because the business of the engine is to give its results in numerical notation, the nature of its processes must consequently be arithmetical and numerical rather than algebraic and analytical. This is an error. The engine can arrange and combine its numerical quantities exactly as if they were letters or any other general symbols; and in fact it might bring out its results in algebraic notation were provisions made accordingly.*

Ada Lovelace, 1815–1852

In the associated problem sheet, we use symbolic computing to

- derive the equations for the orbit of the Earth around the Sun;



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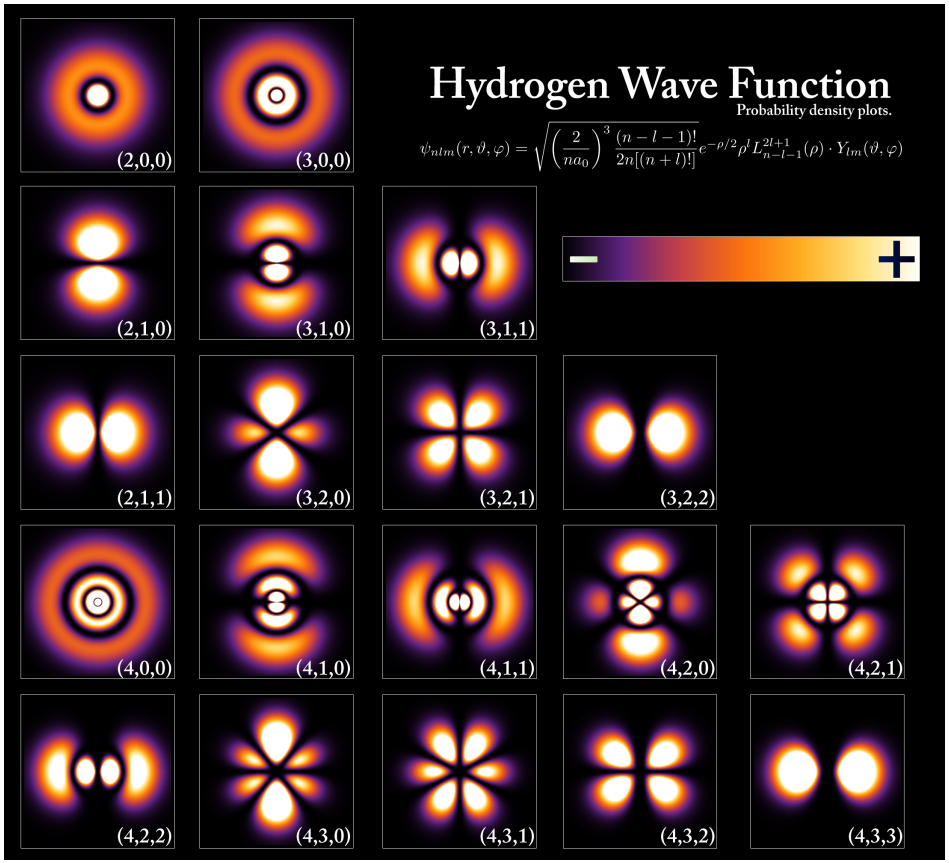
- derive the equations for the orbit of the Earth around the Sun;
- explore the wave function of the hydrogen atom.

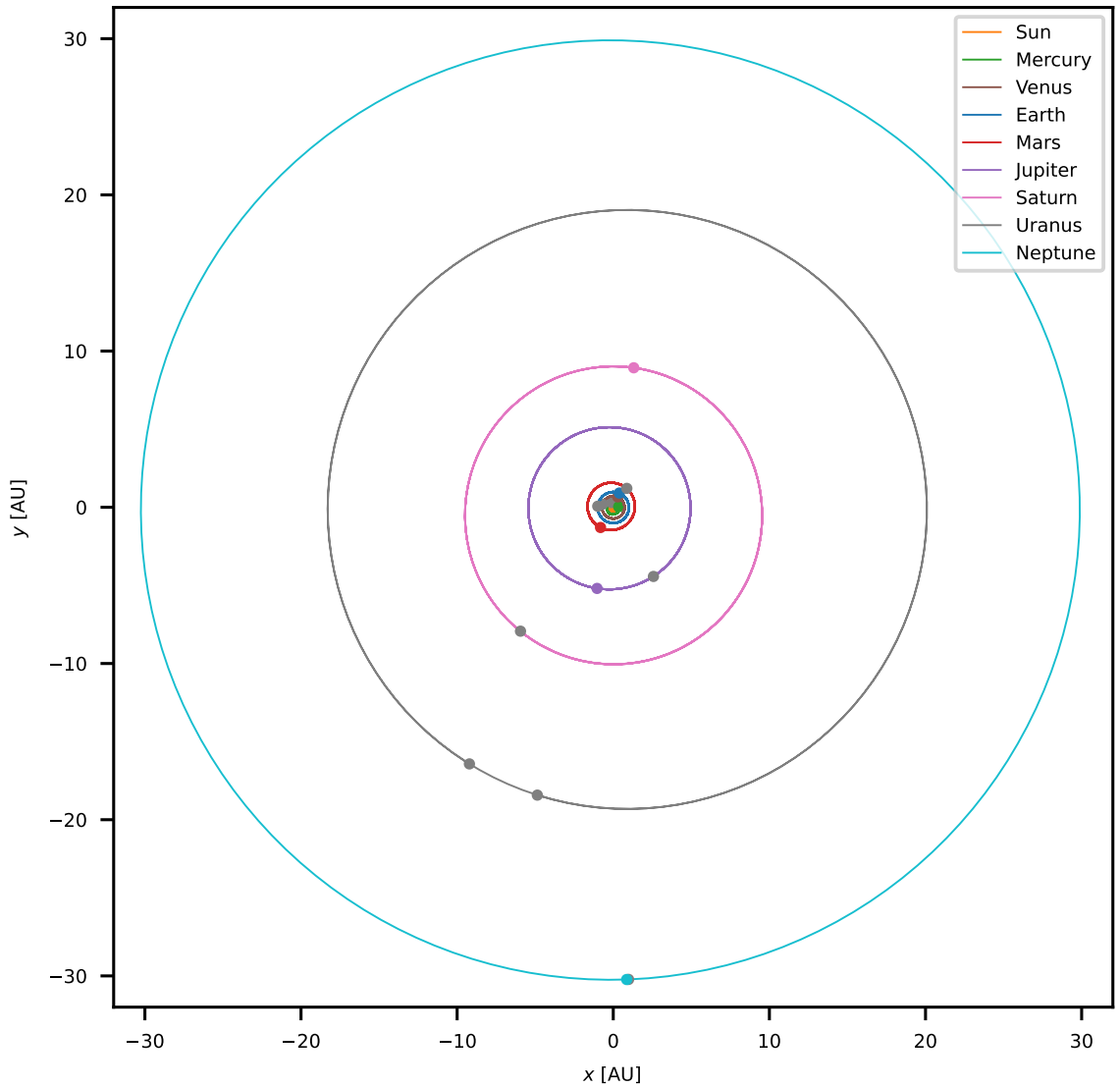


Week 1–2 HT introduces *numerical* computing, a powerful expansion of the conception of what it means to solve a mathematical problem.

We will study

- numerical linear algebra,
- numerical quadrature of integrals,
- least squares and curve-fitting,
- numerical solution of ODE initial value problems.

Week 1–2 HT ends with a code for numerically simulating the solar system.



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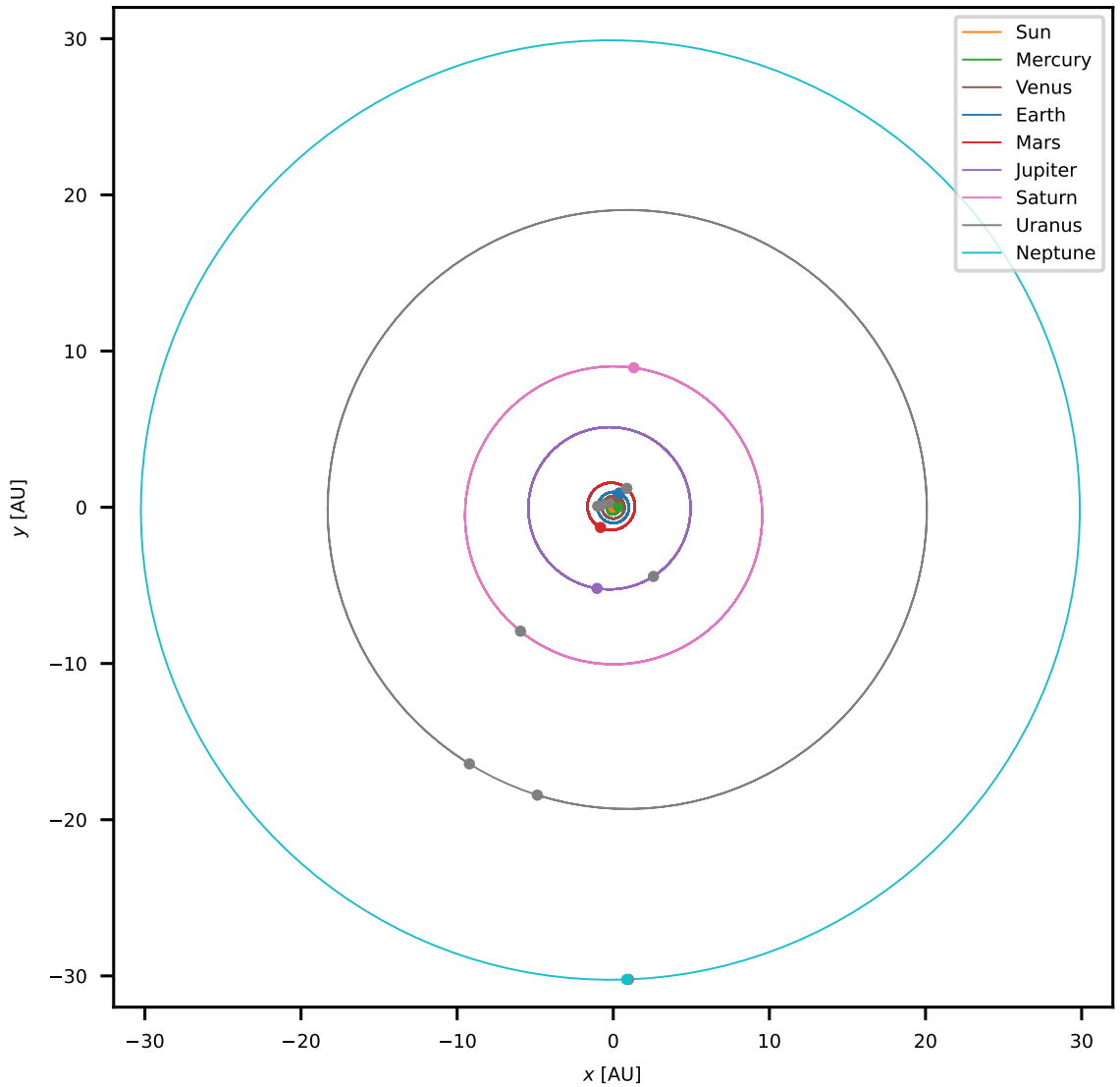


→ `solar.py`

Section 3

# Software installation

$\rightarrow$ Windows

# Computational Mathematics
# Projects

Patrick E. Farrell

University of Oxford

Section 1

# Overview

Computational Mathematics is assessed by projects.

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Passing Computational Mathematics is necessary to pass Prelims.

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- $1^{\text{st}}$ project: 12 noon on Monday of week 6 HT24 (19 Feb)

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Please submit online via Inspera before these deadlines.

The University imposes mark penalties for late submission.

In weeks 1 and 2, the course continues the same as last term.
Demonstrator sessions are scheduled according to college, to support you in completing the final problem sheet.

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After that, there are drop-in demonstrator sessions, open to students of any college:

- Weeks 3–8: Monday 3pm–4pm, and Thursday 3pm–4pm
- Week 5: Wednesday 3pm–5pm, and Friday 3pm–5pm.
- Week 8: Friday 3pm–5pm.

All drop-in sessions are in C1, except for W7 Thursday in C2, W8 Thursday in TCC.

Section 2

# General advice on projects

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Use `publish` to generate a .html of the code and its output.

Submit both your code (.py) and the published output (.html), gathered into exactly one .zip or .tar.gz file.

Examiners may wish to run your code to e.g. test if a function is implemented correctly.

New in HT: you can now do

(terminal) `python publish.py myscript.py`

to generate `myscript.html`.

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to generate `myscript.html`.

This is more efficient than using

(python)
```
from publish import publish; publish()
```

What makes a good submission?

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Projects are marked for mathematics, computing, and clarity of presentation.

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Markers are looking for:

- clear and well-written code;
- computational evidence that each function is correct;
- clear and comprehensible plots (e.g. axis labels, titles, legends);
- mathematical discussion that indicates an understanding of the algorithms and observed results.

We strongly recommend you complete and upload them in good time.

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You may have unforeseen problems with

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- hardware issues, e.g. your computer failing;
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Keep good backups of all your work.

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The University's plagiarism policy applies in full. Potential penalties for plagiarism range from deduction of marks to expulsion.

Section 3

# Project A: primality testing

In 1801, in his magnum opus *Disquisitiones Arithmeticae*, Gauss wrote

> *The problem of distinguishing prime numbers from composite numbers and of resolving the latter into their prime factors is known to be one of the most important and useful in arithmetic. It has engaged the industry and wisdom of ancient and modern geometers to such an extent that it would be superfluous to discuss the problem at length. ... Further, the dignity of the science itself seems to require that every possible means be explored for the solution of a problem so elegant and so celebrated.*

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At Gauss' suggestion, in this project you will explore algorithms for primality testing.

The first step in the Rivest–Shamir–Adleman (RSA) cryptosystem, and many others, is to choose two large primes $p$ and $q$ (secret), and compute $n = pq$ (public).

Ron Rivest, 1947–

Adi Shamir, 1952–

Leonard Adleman, 1945–

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To choose $p$ and $q$, the standard method is to keep choosing random integers until a primality test passes.

Ron Rivest, 1947–

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In 1202, in the *Liber Abaci*, Leonardo of Pisa (Fibonacci) gave the first algorithm for determining whether a number $n \in \mathbb{N}$ is prime, trial division.

> *If it is even, then he recognises its composition. However if odd, then it will be composite or prime. ... Always he goes on dividing in order by prime numbers until he will find a prime number by which he can divide, and thence he will come to the square root; if he will be able to divide by none of them, then one will judge the number to be prime.*

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Can we do better than trial division?

Yes, we can do better than trial division.

Pierre de Fermat, 1607–1665

Gary Miller, ?–

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No composite number is known that falsely passes this test. The construction of such a composite number, or a proof that no such number exists, would solve a major open question in computational number theory.

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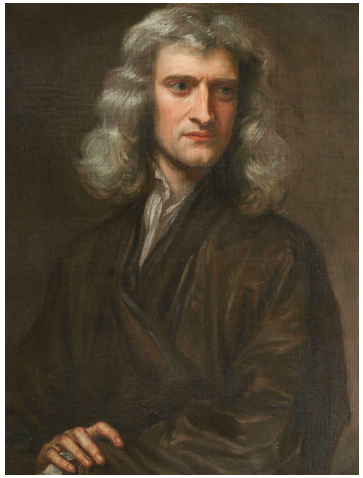
Section 4

# Project B: the Kepler problem

The glorious triumph of Newton's twin discoveries of calculus and Newtonian mechanics was that it allowed us to make *physical predictions* by *solving differential equations*.



Isaac Newton, 1643–1727

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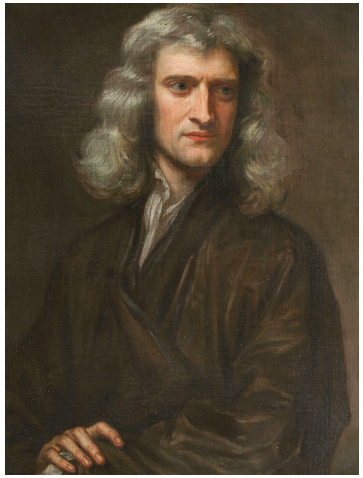
Newton's second law provides an initial value problem for a second-order differential equation that describes the motion of a given system for all future time.



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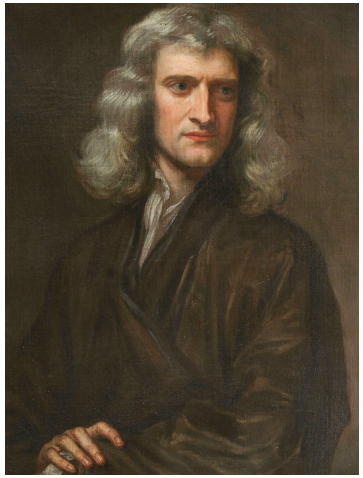

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This tradition continues to this day; *all* of our physical theories are encoded in differential equations:

| Theory | Differential equation |
|---|---|
| Classical mechanics | Hamilton equations |
| Electromagnetism | Maxwell equations |
| Fluid mechanics | Navier–Stokes equations |
| Quantum mechanics | Schrödinger equation |
| General relativity | Einstein field equations |

However, *almost all differential equations* cannot be solved by hand!

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Euler proposed the first useful scheme for the numerical solution of initial value problems in 1768, the forward Euler method, in *Institutiones Calculi Integralis*.

Leonhard Euler, 1707–1783

In this project you will investigate algorithms for the numerical solution of differential equations, in the context of the Kepler problem.

Johannes Kepler, 1571–1630

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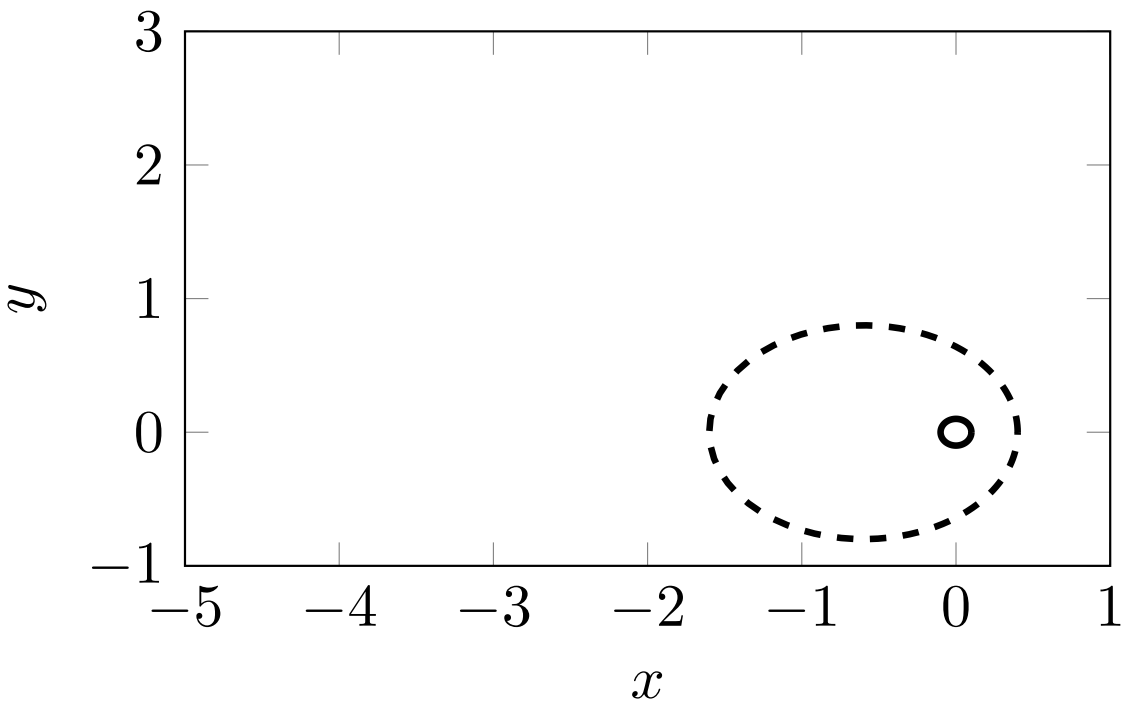

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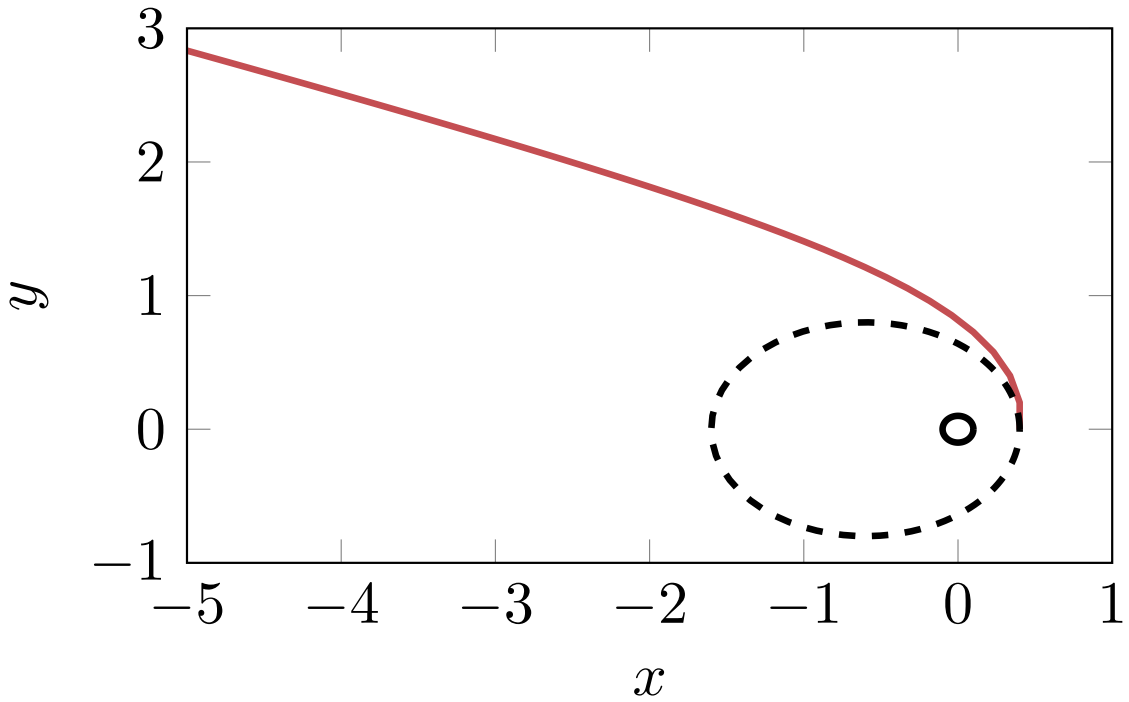

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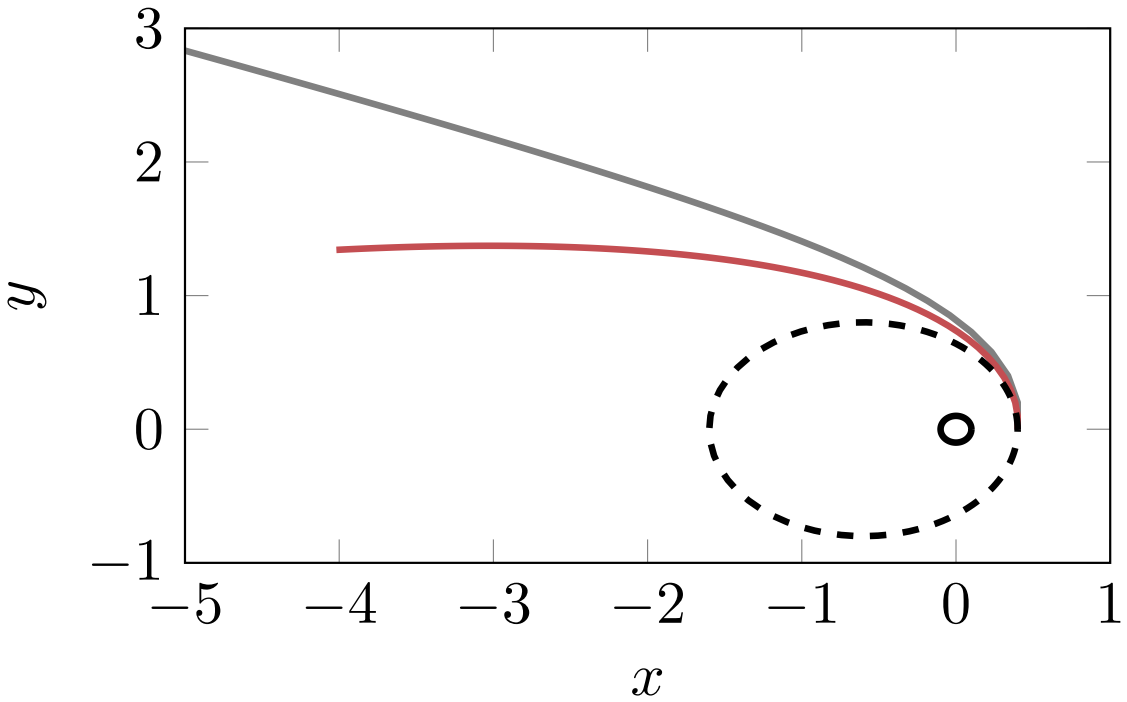


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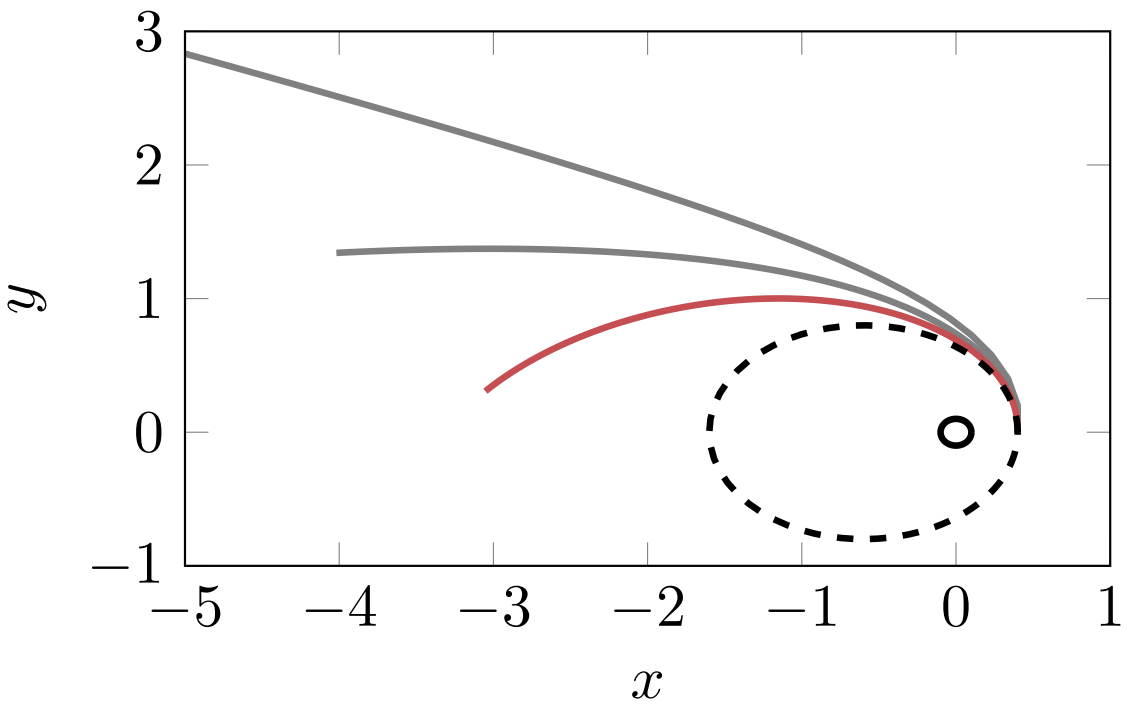


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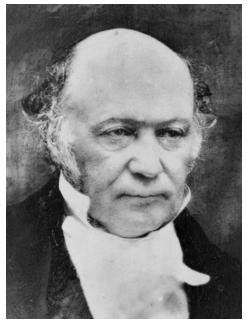

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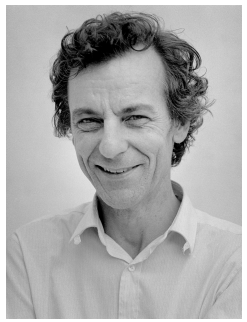

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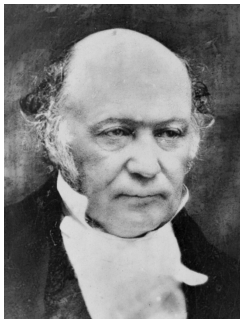

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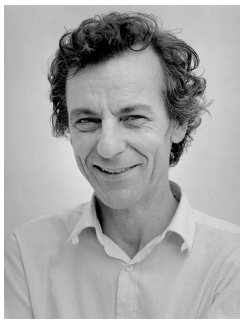

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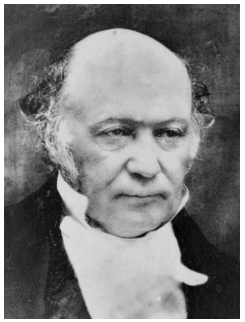

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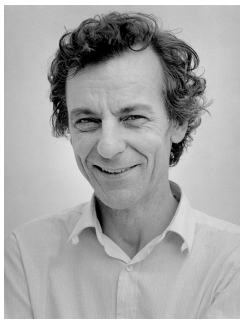

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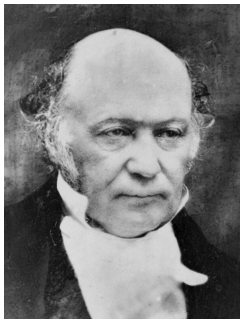
Such methods are essential for accurate long-term simulations of the solar system or understanding the molecular dynamics of complex materials.



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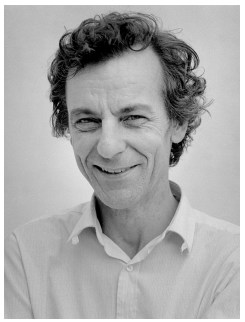

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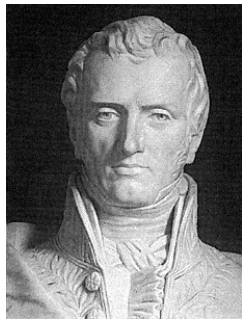

Claude–Louis Navier, 1785–1836

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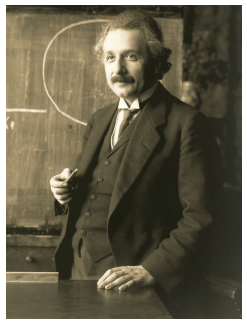

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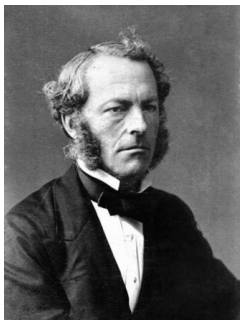

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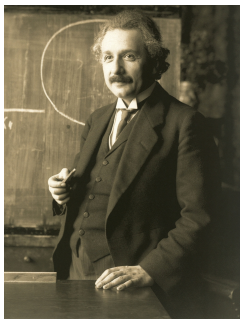

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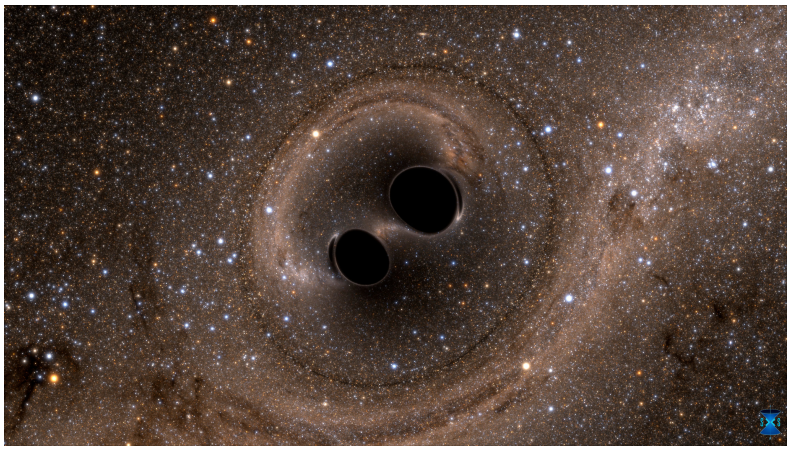
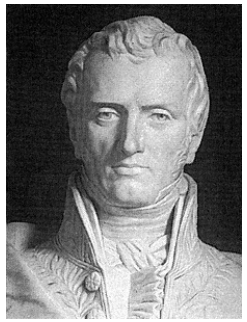


Research in this area allows us to simulate phenomena such as the merger of two black holes.



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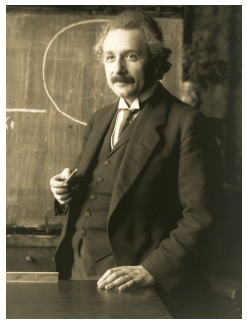

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Section 5

# Project C: percolation

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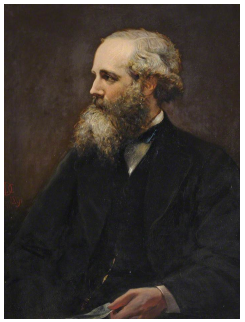
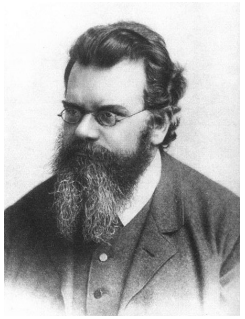
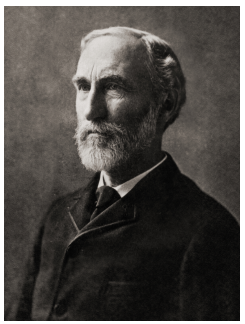


James Clerk Maxwell, 1831–1879



Ludwig Boltzmann, 1844–1906



Josiah Willard Gibbs, 1839–1903

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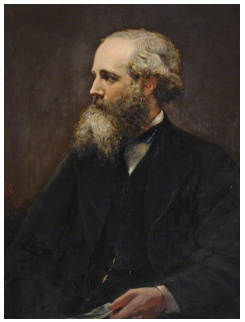
For example, the Newtonian approach to understanding a gas would be to track the velocity and position of each of the trillions of trillions of molecules in a typical cubic metre.



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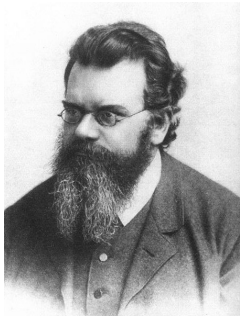

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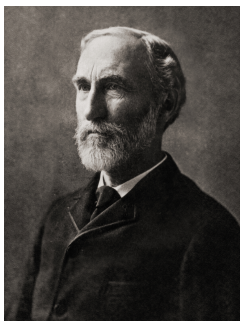

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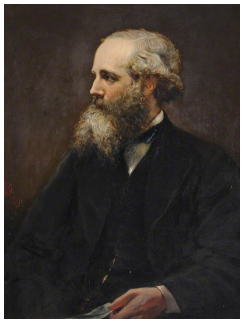
Maxwell's great insight was that this description was excessive. To understand the macroscopic properties of the gas like its pressure or temperature, you could instead merely store a *probability distribution* recording statistics about the molecules.



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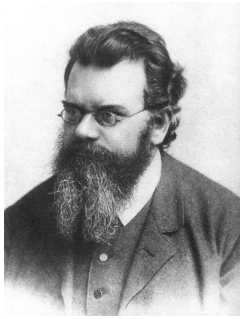

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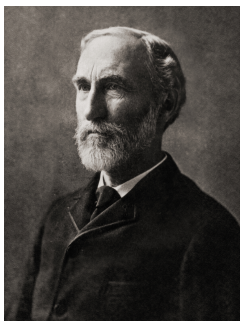

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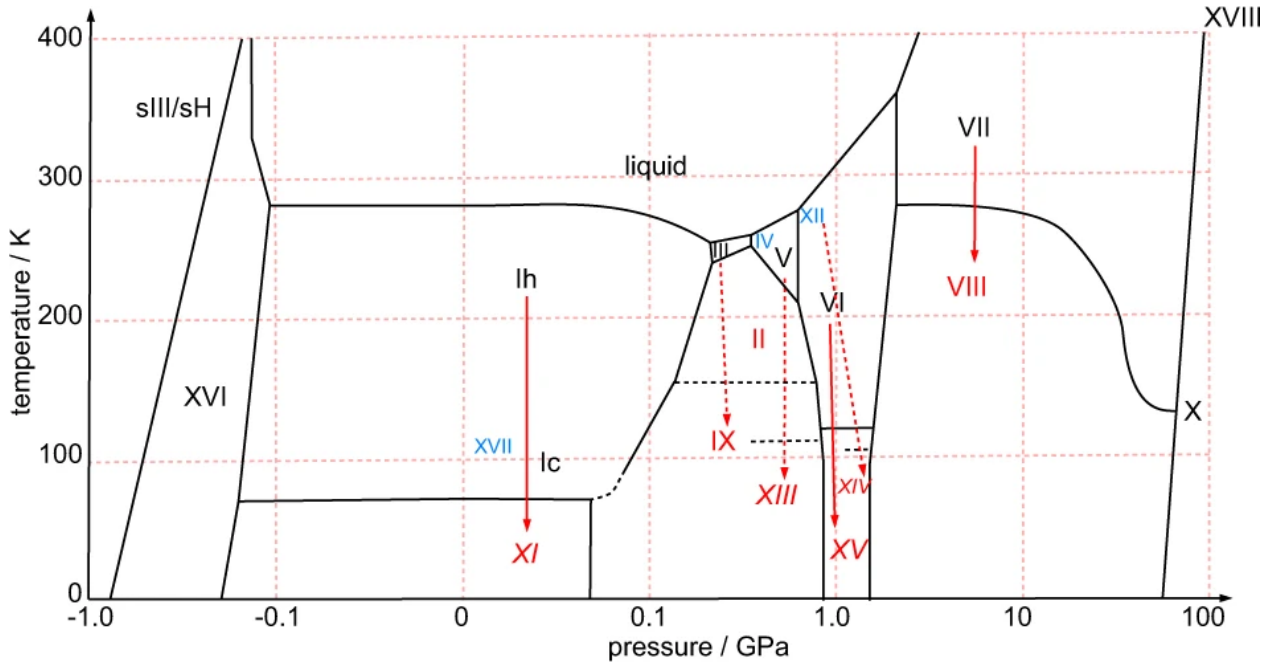


Phase diagram of ice, from Hansen (2021).

Several phases of $H_2O$.

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John Hammersley, 1920–2004

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Percolation theory is active to this day. Hugo Duminil-Copin won a Fields Medal in 2022 for his work in this area.

John Hammersley, 1920–2004

Hugo Duminil-Copin, 1985–

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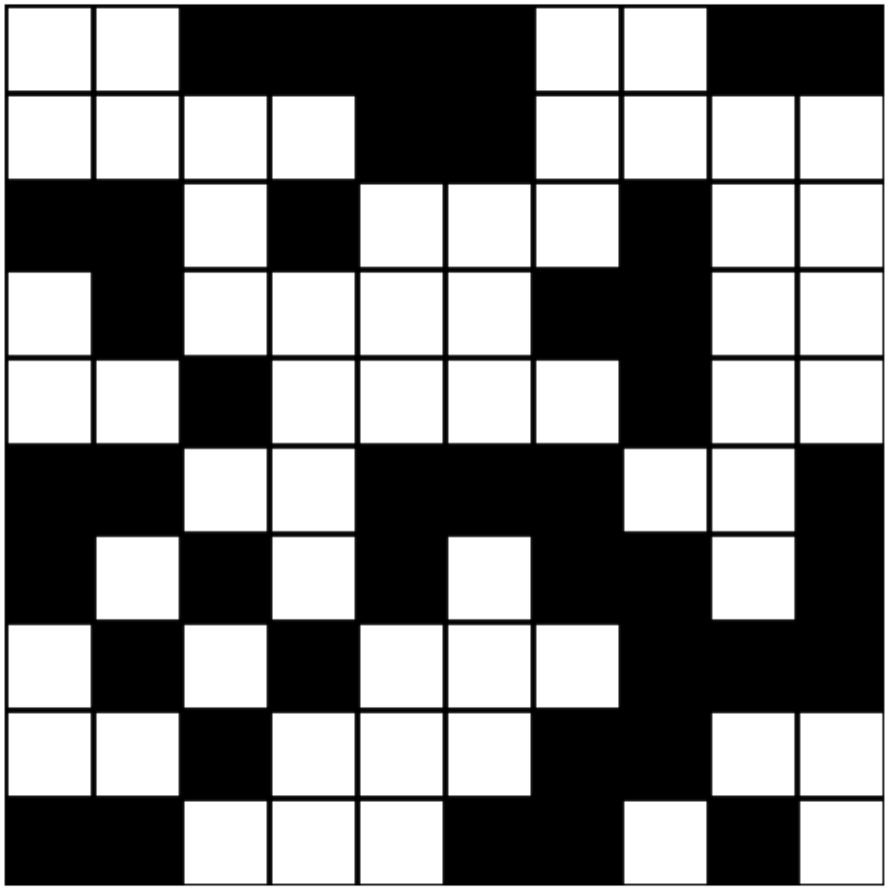

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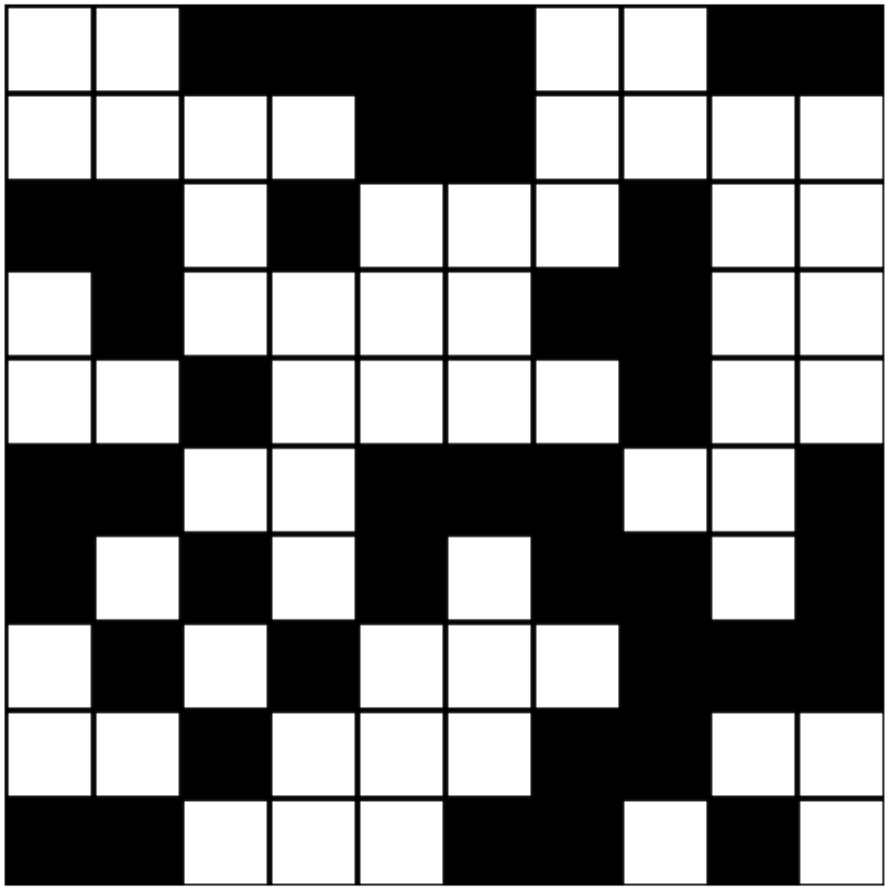

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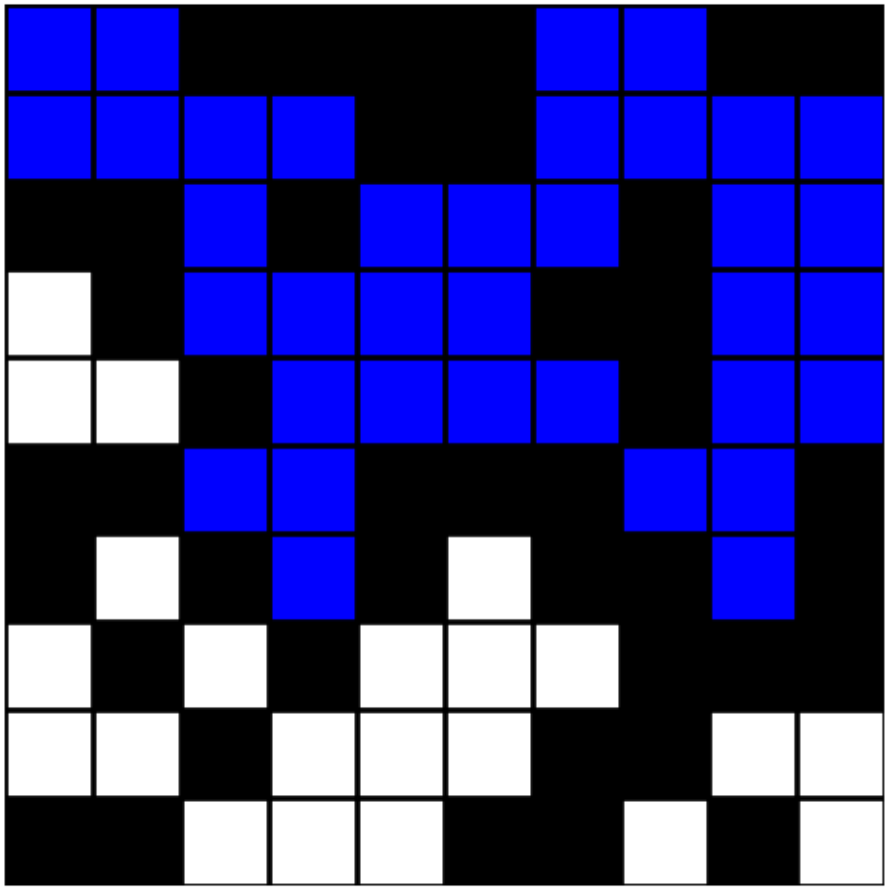

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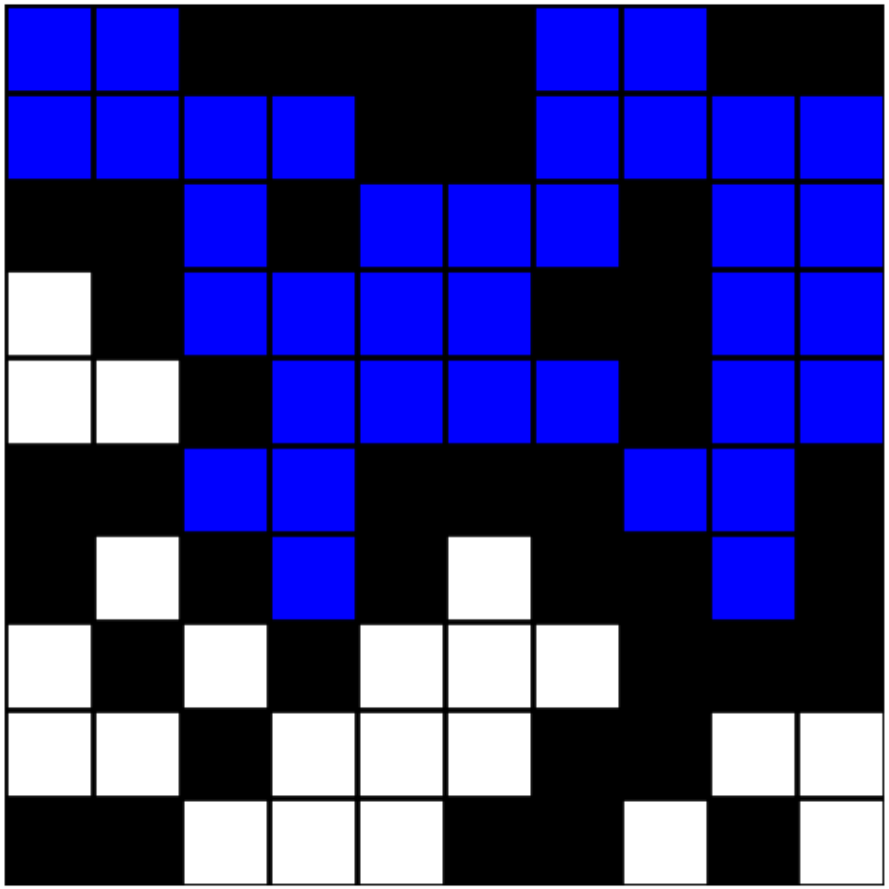

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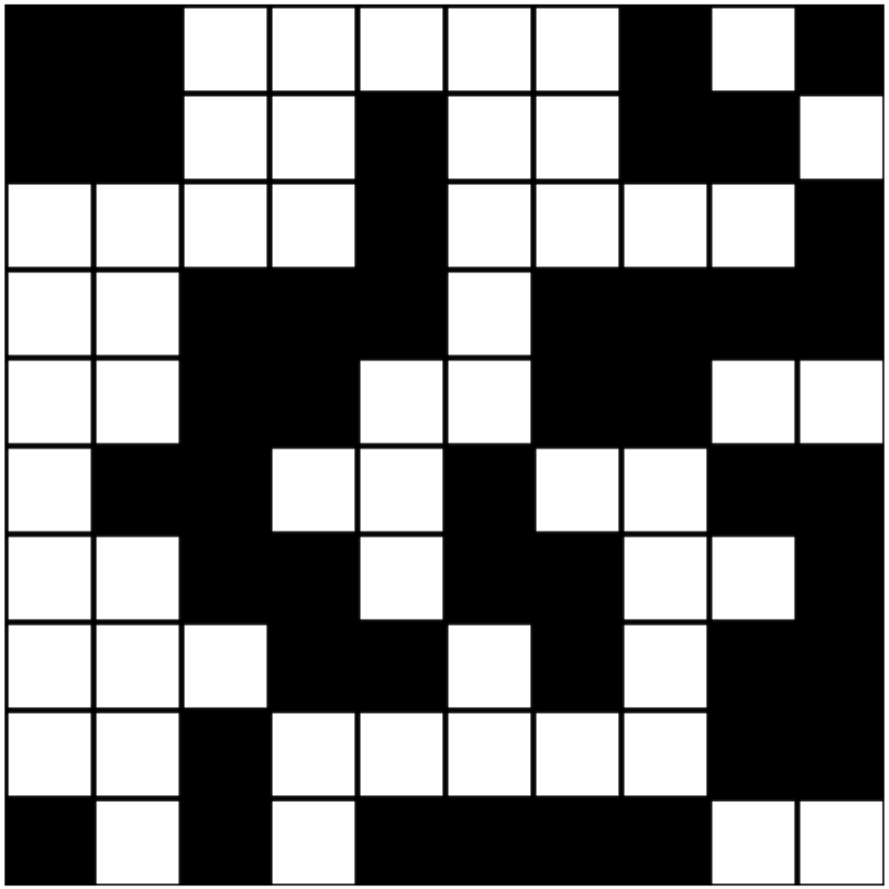

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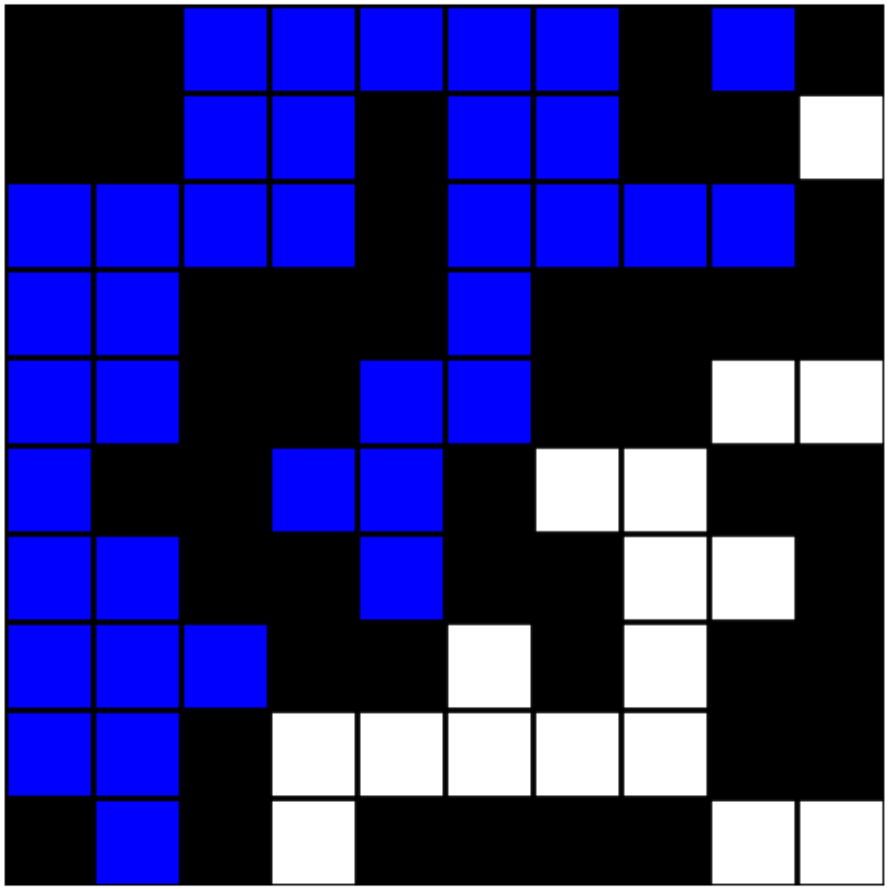

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Despite a great deal of effort, no analytical formula is known for the critical probability $p_c$.

To estimate $C(p)$, we use *Monte Carlo methods*.

Stanisław Ulam, 1909–1984

John von Neumann, 1903–1957

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> *The first thoughts and attempts I made to practice were suggested by a question which occurred to me in 1946 as I was convalescing from an illness and playing solitaires. The question was what are the chances that a Canfield solitaire laid out with 52 cards will come out successfully? After spending a lot of time trying to estimate them by pure combinatorial calculations, I wondered whether a more practical method than "abstract thinking" might not be to lay it out say one hundred times and simply observe and count the number of successful plays.*

Stanisław Ulam, 1909–1984

John von Neumann, 1903–1957

Section 6

# Summary

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- the Kepler problem;
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I hope that you find the projects interesting, and that you have fun!