Computational Mathematics
2026 Projects

Patrick E. Farrell

University of Oxford

Section 1

Overview

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Passing Computational Mathematics is necessary to pass Prelims.

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The University imposes mark penalties for late submission.

Section 2

General advice on projects

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Each project has some mathematical questions not answered by coding. You can write your answer in words, or use basic latex: adding

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to your code produces published output that looks like

$$\sin x = 1.$$

You can write latex inline using dollars: \$\sin{x}\$ produces $\sin x$.

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

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

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

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Projects are marked for mathematical insight (40%), programming skill (40%), and clarity of presentation (20%).

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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 understanding of and insight into the algorithms and observed results.

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

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

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When you do these, include the URL of the resource you have employed in code comments, as a citation.

Section 3

2026A: topological classification

Geometry

Study properties of a shape like lengths, angles, areas, volumes—all induced by a *metric*.

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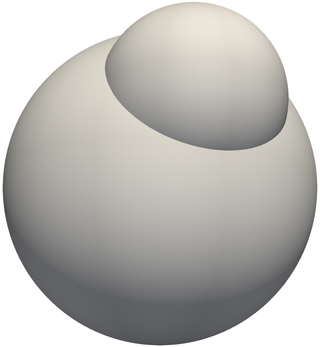
Study properties of a shape that are independent of the metric, those preserved under *homeomorphism*.

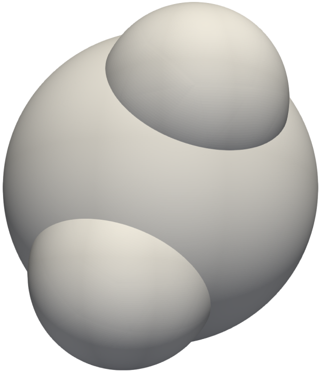
Definition (Homeomorphism)

A homeomorphism is a continuous bijection with continuous inverse.

(a)

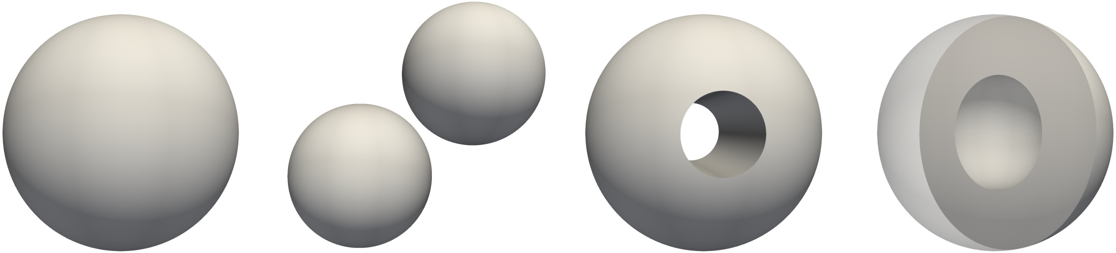


(b)



(c)

Three homeomorphic manifolds.



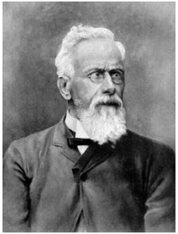
(a) a solid sphere (b) two solid spheres (c) solid sph. with a tunnel (d) solid sph. with a void

Four manifolds, none of which are homeomorphic to any other.

Classification

How can we classify different manifolds, so that

$$\text{different class} \implies \text{not homeomorphic?}$$



Enrico Betti, 1823–1892

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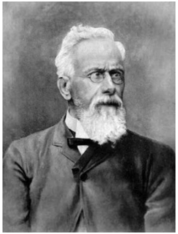

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The Betti numbers

Count the number of 'k-dimensional holes'.

We will define the Betti numbers in the project. But in low dimensions we can understand them as

- b_0 the number of connected components (separate pieces),
- b_1 the number of tunnels (where light could pass from one side to the other),
- b_2 the number of voids (where you could store water as the body rotates).

Betti numbers:

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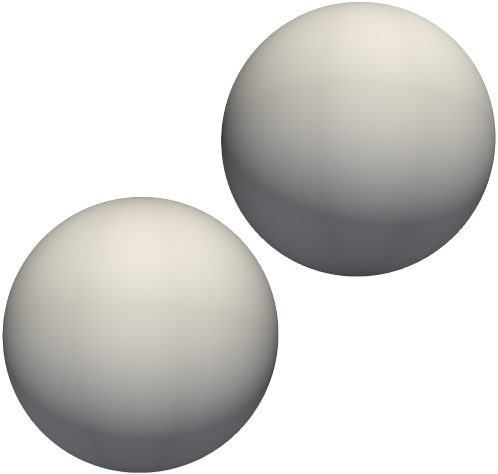

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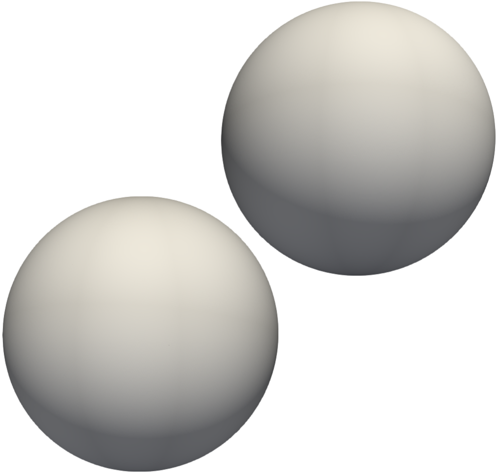
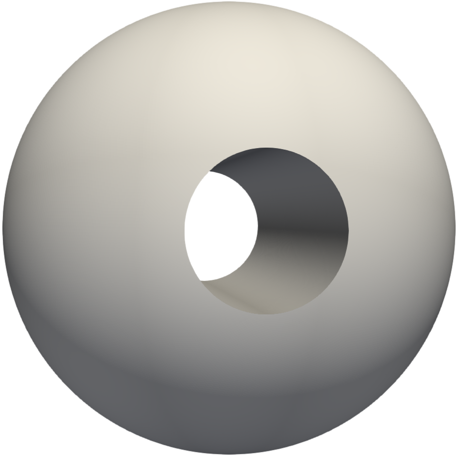


Betti numbers: $(b_0, b_1, b_2) = (2, 0, 0)$



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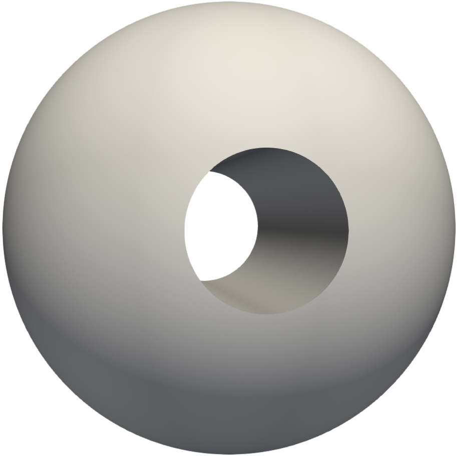
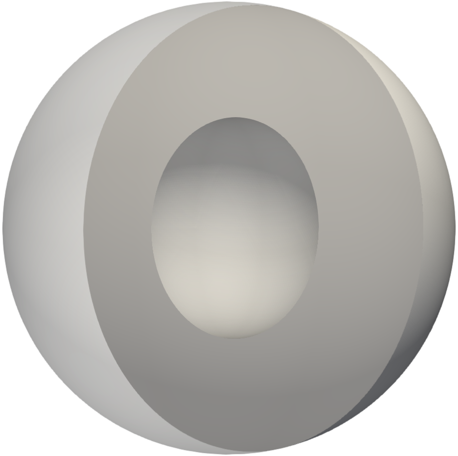


Betti numbers: $(b_0, b_1, b_2) = (1, 1, 0)$



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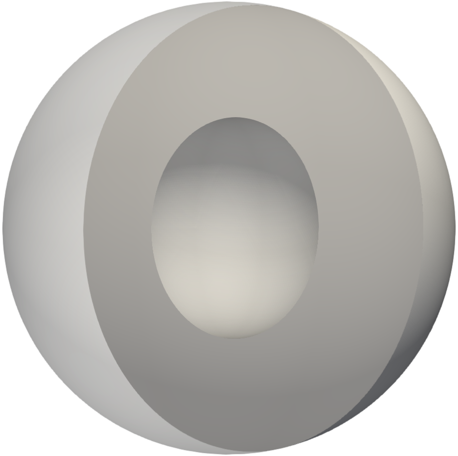

Betti numbers: $(b_0, b_1, b_2) = (1, 0, 1)$

So how can we compute Betti numbers?

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Simplicial homology

Triangulate the domain into oriented *simplices* and use linear algebra.

Henri Poincaré, 1854–1912

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Simplicial homology

Triangulate the domain into oriented *simplices* and use linear algebra.

We can study the topological properties of something *continuous* with something *discrete*.

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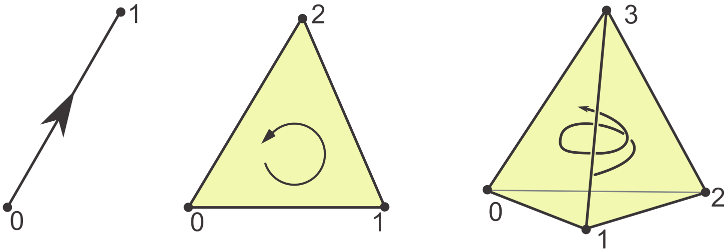
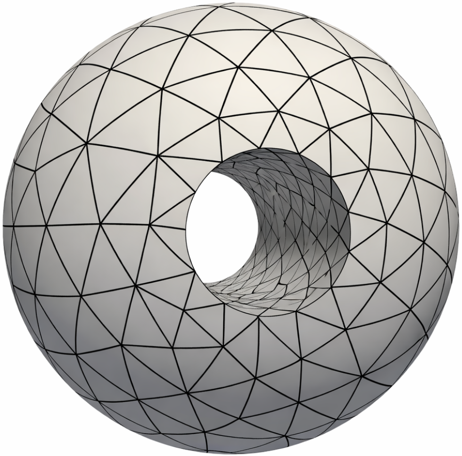


Definition (a k-simplex)

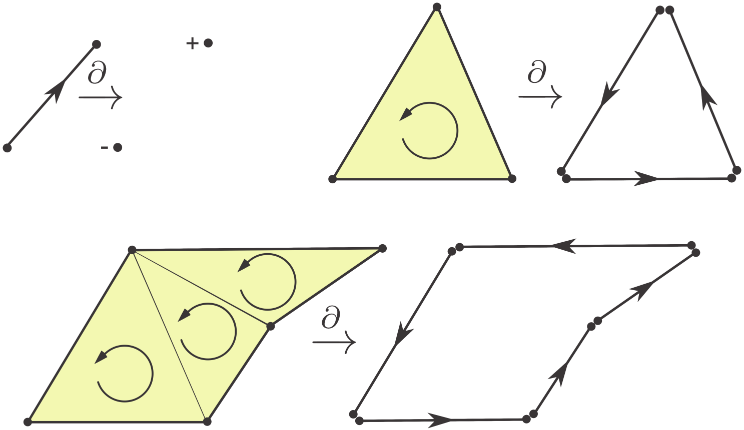
A k-simplex is the convex hull of $k+1$ independent points.



A simplicial complex.

The boundary of a set of $(k+1)$-simplices ...

...is a set of k-simplices.



Fundamental principle

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So we have

$$\mathrm{im}(\delta_{k+1}) \subseteq \ker(\delta_k)$$

but is

$$\mathrm{im}(\delta_{k+1}) = \ker(\delta_k)?$$

Surprising fact

It depends on the topology of the domain!

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Poincaré's insight was that the Betti numbers can be calculated by quantifying how much

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differ.

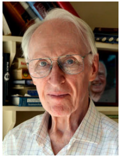
In this project you will use this to calculate the Betti numbers of a given manifold.

Some consider the relation

$$\delta_k \circ \delta_{k+1} = 0$$

to be one of the mathematical foundations of reality.

> *...Thus simply is all of general relativity tied to the principle that the boundary of a boundary is zero. No one has ever discovered a more compelling foundation for the principle of conservation of momentum and energy. No one has ever seen more deeply into that action of matter on space, and space on matter, which one calls gravitation. In summary, the Einstein theory realizes the conservation of energy-momentum as the identity, "the boundary of a boundary is zero."*



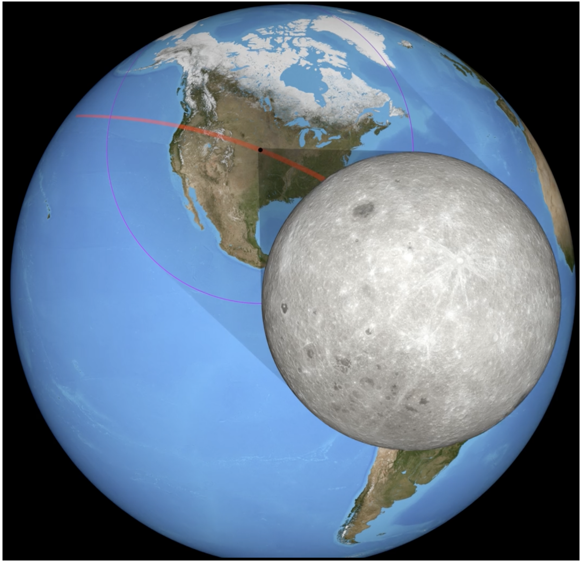
Charles Misner, 1932–2023

Kip Thorne, 1940–

John Wheeler, 1911–2008

Section 4

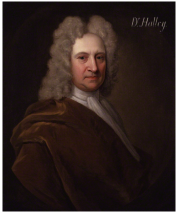
2026B: predicting eclipses



Eclipses have always held special meaning for humans.

Tablet K.2600, on display in the British Museum. This fragment, combined with several others, describes the Neo-Assyrian ritual for appointing a sacrificial king.

In 1715, Halley published a map predicting the path of an eclipse over London, two weeks before it happened.



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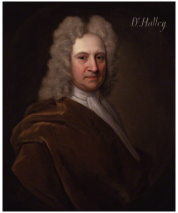
> *The like Eclipse having not for many Ages been seen in the Southern Parts of Great Britain, I thought it not improper to give the Publick an Account thereof, that the suddain darkness, wherin the Starrs will be visible about the Sun, may give no surprize to the People, who would, if unadvertized, be apt to look upon it as Ominous, and to Interpret it as portending evill to our Sovereign Lord King George and his Government, which God preserve.*



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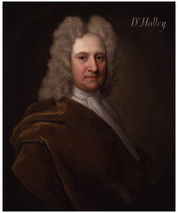
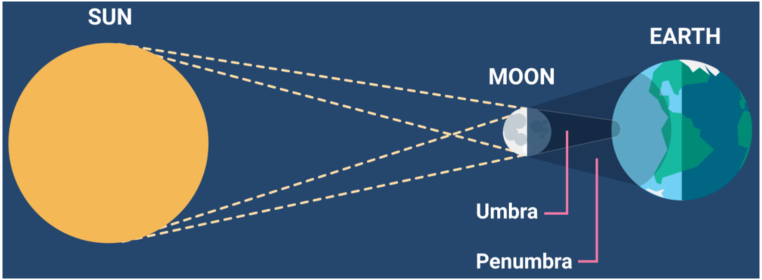
This was a dramatic public vindication of Newton's theory of gravity.



Edmund Halley, 1656–1742


10. April. 1715.
A Defcription of the Pafsage of the Shadow of the Moon, over England,
In the Total Eclipse of the SUN, on the 22d Day of April 1715 in the Morning.
A Scale of 60 computed Miles
THE GERMAN SEA
SCOTLAND
THE IRISH SEA
IRELAND
St. GEORGE'S CHANNEL
THE CHANNEL
FRANCE
Firth of Forth
I. Wight
Engrav'd by John Senex

In this project you will learn how to predict the paths of eclipses using the *Besselian elements*.

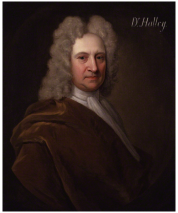


Friedrich Bessel, 1784–1846

The Besselian elements are a set of coefficients for polynomial functions of time that describe the geometry of the umbral and penumbral cones.

From this time the Eclipse advanced, and by Nine of the Clock was about Ten Digits, when the Face and Colour of the Sky began to change from perfect serene azure blew, to a more dusky livid Colour having an eye of Purple intermixt, and grew darker and darker till the total Immersion of the Sun, which happened at $9^h 9' \cdot 17''$ by the Clock ...

This Moment was determinable with great nicety, the Sun's light being extinguish'd at once; and yet more so was that of the Emersion, for the Sun came out in an Instant with so much Lustre that it surprized the Beholders, and in a Moment restored the Day.



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Section 5

2026C: irreversibility from reversible dynamics

Observation

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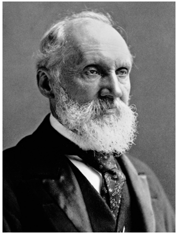
...why does the future not look like the past? Why does time go forwards and not back?

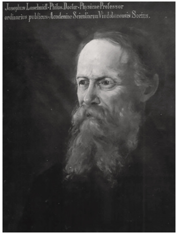
Why does the universe exhibit phenomena that are *irreversible*?

If, then, the motion of every particle of matter in the universe were precisely reversed at any instant, the course of nature would be simply reversed forever after. The bursting bubble of foam at the foot of a waterfall would reunite and descend into the water; the thermal motions would reconcentrate their energy and throw the mass up the fall in drops re-forming into a close column of ascending water ...Boulders would recover from the mud the materials required to rebuild them into their previous jagged forms, and would become reunited to the mountain peak from which they had formerly broken away. And if, also, the materialistic hypothesis of life were true, living creatures would grow backward, with conscious knowledge of the future but with no memory of the past, and would become again, unborn.

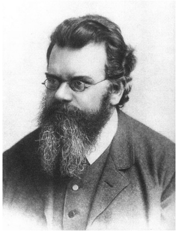


William Thomson, 1824–1907

This problem is known as Loschmidt's paradox, who raised the objection soon after Boltzmann's proof that the Boltzmann equation is irreversible.



Josef Loschmidt, 1821–1895



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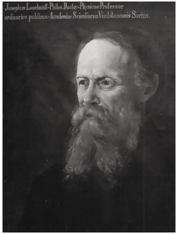

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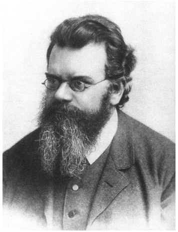

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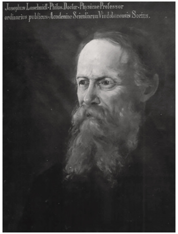

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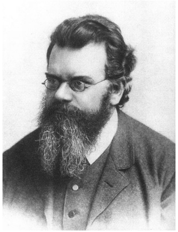

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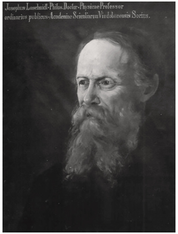
This is quantified by the second law of thermodynamics, which states that the *entropy* of an isolated system can never decrease. It is the second law that provides an inequality, and gives a direction to the 'arrow of time'.



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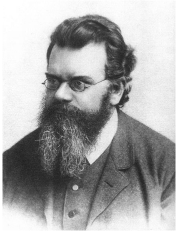

Ludwig Boltzmann, 1844–1906

In 1956 Mark Kac proposed the Kac ring, an extremely simple model with

(i) perfectly reversible microscopic dynamics, and

(ii) irreversible macroscopic dynamics.

Mark Kac, 1914–1984

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In this project we will build intuition for the standard resolution of Loschmidt's paradox using the Kac ring.

Mark Kac, 1914–1984

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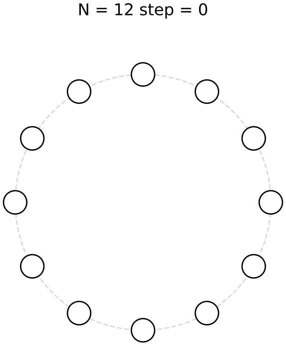
Each site has a white ball or black ball.



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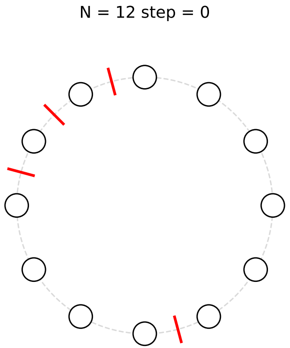

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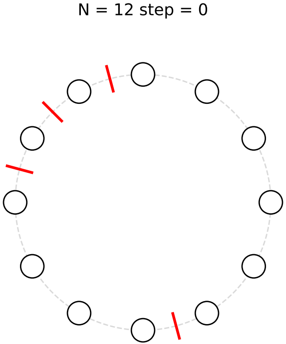

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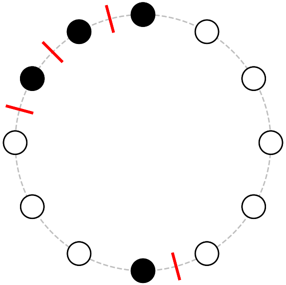

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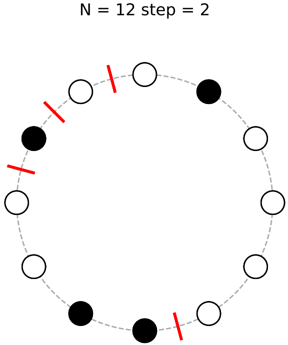

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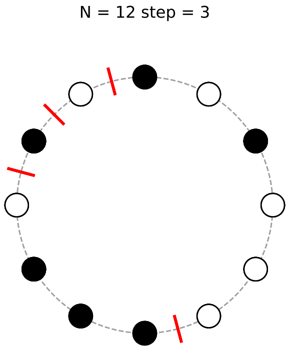

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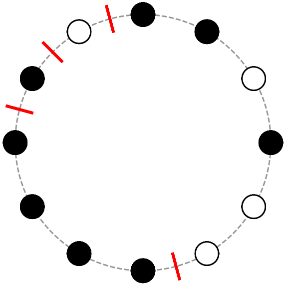

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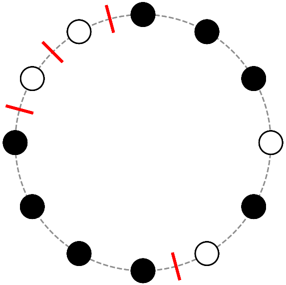

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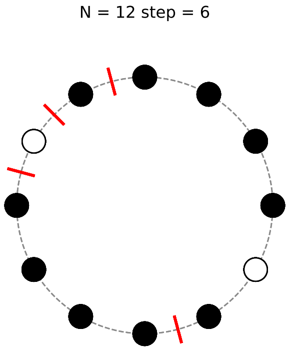

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Observation principle

We think of W and B as *macroscopic* properties that are observable, but w and b are *microscopic* properties that are not observable. We can only measure the *coarse-grained* system.

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Note that we *cannot eliminate* w and b from the evolution law.

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Closure assumption

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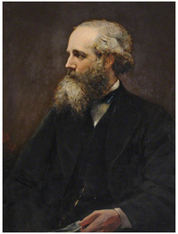

James Clerk Maxwell, 1831–1879

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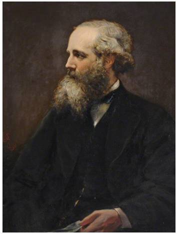
In statistical mechanics, this assumption is called the *molecular chaos assumption*, proposed by Maxwell in 1860.



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Another surprising conclusion

The second law of thermodynamics arises because of this microscale-macroscale distinction: *entropy measures the degree of non-injectivity of our coarse-graining*.

As Carlo Rovelli puts it,

> *Boltzmann has shown that entropy exists because we describe the world in a blurred fashion. He has demonstrated that entropy is precisely the quantity that counts how many are the different configurations that our blurred vision does not distinguish between. ...*
>
> *This is the disconcerting conclusion that emerges from Boltzmann's work: the difference between the past and the future refers only to our own blurred vision of the world. It's a conclusion that leaves us flabbergasted: is it really possible that a perception so vivid, basic, existential—my perception of the passage of time—depends on the fact that I cannot apprehend the world in all of its minute detail?*

Carlo Rovelli, 1956–

Section 6

Summary

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- predicting eclipses;
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Valediction

I hope that you find the projects interesting and enjoyable!

Section 7

Previous projects: comments and guidance

Section 8

2024A: 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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In this project we explored algorithms for primality testing.

Question 2024A.1. Modify your code for Exercise 7.6 (which implements an efficient variant of trial division) to return `(flag, ndivisions)`, where `flag = True` if the input is prime and `False` otherwise, and `ndivisions` is the count of the number of divisions performed. Print the output of the function applied to all $n \in 2:20$. How many divisions are performed to test the primality of 9999991111111?

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$\longrightarrow$ code

Many answers didn't correctly count the number of divisions performed:

```
for m in range(2, math.isqrt(n)):
    if m == 2 or m == 3 or m % 6 == 1 or m % 6 == 5:
        ndivisions += 1
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Some answers missed the point completely and tested with each odd number, or worse, with each number up to $\sqrt{n}$.

Question 2024A.2. Compute the number of divisions performed for all numbers $n \in 2 : 10^5$. By means of a plot, verify that trial division takes about $\sqrt{n}/3$ divisions in the worst case to test a number n for primality.

The code for the first question already returns the number of divisions required:

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N = list(range(2, 10**5+1))
divisions = [trial_division(n)[1] for n in N]
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The very best answers (not necessary for full marks) commented that the number of inputs requiring the maximum number of divisions (i.e. prime numbers) appears not to decrease over time—this is because the Prime Number Theorem guarantees that

$$\frac{\pi(n)}{n} \sim \frac{1}{\log n}$$

which decays slowly.

Question 2024A.3. Write a function to implement the Fermat trial for given n and a. Write another function to apply the Fermat test with all a in a given list; if no list is supplied, use as default value all $a \in 2 : (n-2)$ in ascending order. This latter function should return a tuple `(flag, ntrials)` where `flag = False` if the Fermat test has shown n to not be prime and `True` otherwise[1], and where `ntrials` is the number of Fermat trials performed. Print the output of the function applied to the natural numbers $n \in 2 : 20$, using in each case all $a \in 2 : (n-2)$ in ascending order.

[Hint: the greatest common divisor can be computed using `math.gcd`.]

[Hint: in Python, the `pow` function takes an optional third argument. `pow(x, y, z)` calculates $x^y \mod z$.]

[1] In other words, a number with flag `True` might still be composite.

The question explicitly requests two functions. Some answers did not write two functions, or wrote two functions where one did not call the other.

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There was some confusion around how to write functions with default values for variables. Such answers generally used global variables to determine the bases to use, which is fragile, and they often worked incorrectly.

Question 2024A.4. Compute the first 5 odd numbers n where the Fermat test proves compositeness with just one trial, i.e. with $a = 2$.

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This was more or less answered correctly by everyone with a correct implementation of the Fermat test.

Question 2024A.5. For how many odd $n \in 3 : 10,000$ does the Fermat test prove compositeness with at most five trials (using $a \in 2 : \min(6, n-2)$)? What proportion of odd composite numbers in $3 : 10,000$ does this represent?

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Generally answered well. Some students divided by the number of odd numbers, not odd composite numbers.

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Generally answered well. Some students divided by the number of odd numbers, not odd composite numbers.

Some didn't get the loop right and their count was off by one or two.

Question 2024A.6. A *Carmichael number*, also called an absolute Fermat pseudoprime, is a composite number which passes the Fermat trial for any $a \in 2:(n-1)$ with $\gcd(a, n) = 1$. Compute the Carmichael numbers up to $10,000$.

[Hint: the first Carmichael number is 561*.]*

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[Hint: the first Carmichael number is 561*.]*

Generally answered well. The very best answers (not needed for full marks) investigated whether the number of Carmichael numbers followed the $n^{\frac{2}{7}}$ law prediced by Alford, Granville & Pomerance.

Question 2024A.7. Write a function to implement the Miller–Rabin trial for given n and a.

Write another function to apply the Miller–Rabin test with all a in a given list; if no list is supplied, use as default value the single trial $a = 2$. This latter function should return a tuple `(flag, ntrials)` where `flag = False` if the Miller–Rabin test has shown n to not be prime and `True` otherwise[2], and where `ntrials` is the number of Miller–Rabin trials performed. Print the output of the function applied to the natural numbers $n \in 5 : 20$, using in each case only $a = 2$.

[2] In other words, a number with flag `True` might still be composite.

The main difficulty here was computing s and d such that

$$n - 1 = 2^s d$$

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```python
# Write $n - 1 = 2^s d$.
s = 0
d = n - 1
while d % 2 == 0:
    s += 1
    d = d / 2
```

```python
assert d == int(d)
d = int(d)
assert n - 1 == 2**s * d
assert d % 2 == 1
```

Question 2024A.8. Using only the single trial with base $a = 2$, what is the minimal odd composite number n for which the test does not conclude that n is composite?

Question 2024A.9. Using only the trials $a \in \{2, 3\}$, what is the minimal odd composite number n for which the test does not conclude that n is composite?

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These questions are very similar, so write one function that takes in the bases to use.

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These questions are very similar, so write one function that takes in the bases to use.

This also makes it easier to test the code on the examples that are given in the question—the question tells us the minimal inconclusive odd composite number for bases $\{2, 3, 5\}$.

Question 2024A.10. Using trials $a \in \{2, 3, 5, 7, 11, 13, 17\}$[3], how much faster or slower is the Miller–Rabin test than trial division to verify the primality of $n = 9999991111111$?

[3] With these bases, the Miller–Rabin test is guaranteed to be correct for this n.

Question 2024A.10. Using trials $a \in \{2, 3, 5, 7, 11, 13, 17\}$[3], how much faster or slower is the Miller–Rabin test than trial division to verify the primality of $n = 9999991111111$?

On Windows, it turns out that the operating system timer isn't fine-grained enough to capture the time taken by a Miller–Rabin trial. (I didn't know this.) Many answers therefore reported a time of 0.0 s.

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Question 2024A.10. Using trials $a \in \{2, 3, 5, 7, 11, 13, 17\}$[3], how much faster or slower is the Miller–Rabin test than trial division to verify the primality of $n = 9999991111111$?

On Windows, it turns out that the operating system timer isn't fine-grained enough to capture the time taken by a Miller–Rabin trial. (I didn't know this.) Many answers therefore reported a time of 0.0 s.

This obviously doesn't make sense. The right thing to do here is to instead time 100 or 1000 trials, and then divide by the number of trials taken, to get a sensible estimate.

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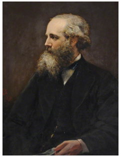
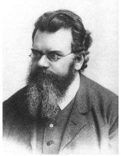
Section 9

2024C: Percolation

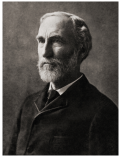
Statistical mechanics, founded by Maxwell, Boltzmann, and Gibbs in the 1800s, applies statistical and probabilistic methods to large assemblies of microscopic entities.



James Clerk Maxwell, 1831–1879



Ludwig Boltzmann, 1844–1906



Josiah Willard Gibbs, 1839–1903

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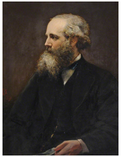
For example, the Newtonian approach to understanding a gas would be to track the velocity and position of each of the trillions of trillions of molecules in a typical cubic metre.



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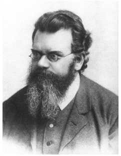

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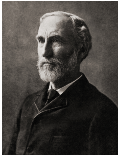

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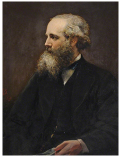
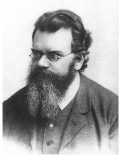
For example, the Newtonian approach to understanding a gas would be to track the velocity and position of each of the trillions of trillions of molecules in a typical cubic metre.

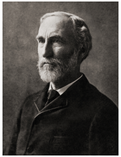
Maxwell's great insight was that this description was excessive. To understand the macroscopic properties of the gas like its pressure or temperature, you could instead merely store a *probability distribution* recording statistics about the molecules.



James Clerk Maxwell, 1831–1879



Ludwig Boltzmann, 1844–1906



Josiah Willard Gibbs, 1839–1903

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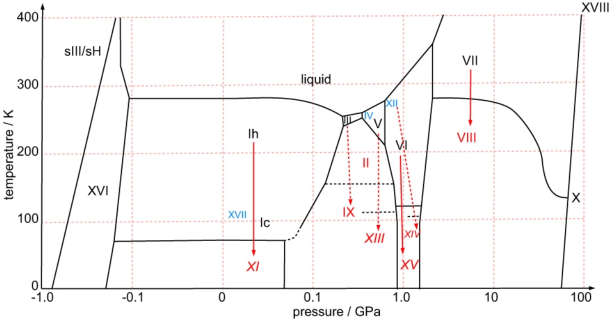

Phase diagram of ice, from Hansen (2021).

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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.

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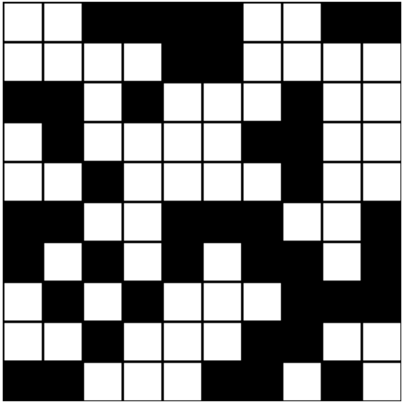

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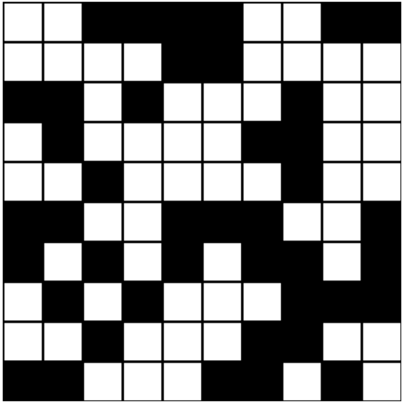

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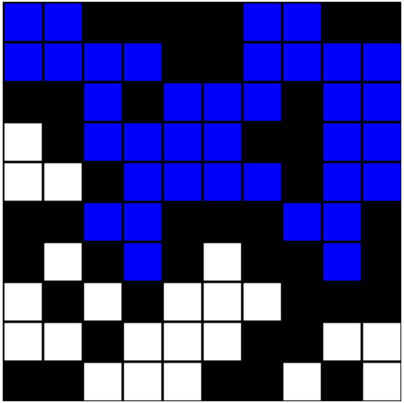

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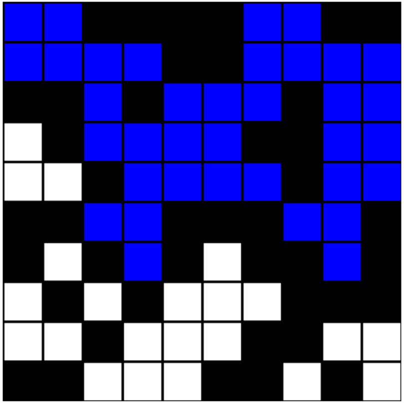

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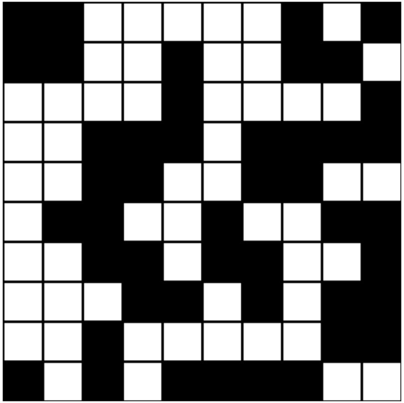

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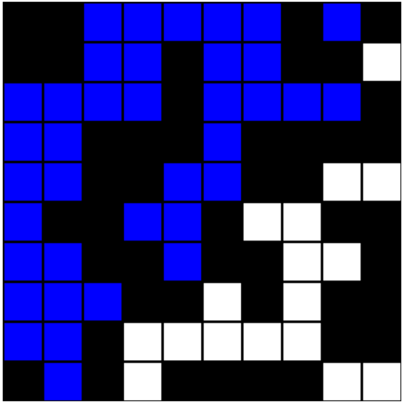

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$C(p)$ jumps very rapidly from 0 to 1 around a critical $p = p_c$.

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*.

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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.*

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Question 2024C.1. Write a function `make_grid(n, p)` to make an $n \times n$ numpy array of Boolean values, with each site `True` with probability p and `False` otherwise.

[Hint: this should take one line of numpy code.]

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Weaker answers computed the mean with manual loops; better answers used `np.mean` or `np.sum`.

Question 2024C.2. Write a function `visualise_grid` to visualise a grid produced by `make_grid` with matplotlib. The function should take in a Boolean array. The output should look similar to [Figure]: plot closed sites in black; plot open sites in white; colour the borders of each square in black.

[Hint: you will need to consult the matplotlib documentation and other online resources to do this; the relevant matplotlib methods were not discussed in the handbook.]

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Use your function to visualise a few sample grids.

Some answers flipped black and white. A few answers flipped up with down. You should print out the grid that you render and check by eye that they conform.

Question 2024C.3. Write a function `visualise_fill` to visualise the fill status of a given grid. The function should take as input two Boolean arrays, the grid and the fill status. The output should look similar to [Figures]. Plot closed sites in black, open unfilled sites in white, and open filled sites in blue. Colour the borders of each square in black.

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My comments here are similar.

Question 2024C.4. Write a function `compute_fill` that takes in a grid produced by `make_grid` and calculates whether each site is full or not.

[Hint: think carefully about what should happen when a site is visited. For example, if it is already full, it should terminate without further action.]

[Hint: it may be useful during your development to visualise the fill state of the grid as you visit each site in the top row.]

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Implementations ranged from very elegant to very convoluted. Some implementations swept through the grid row-by-row, not allowing propagation of fill upwards.

Question 2024C.5. Write a function `percolates` that returns `True` if the given grid percolates, and `False` otherwise.

[Hint: the core logic can be written with one line of numpy.]

Draw 10 samples of a 20×20 grid with vacancy probability $p = 0.6$. For each, visualise its fill status, titling each figure with whether that grid percolates or not.

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A few answers were egregiously inefficient: they called `compute_fill` over and over on each column.

Question 2024C.6. Take a suitable grid $P \subset [0,1]$ of p values. (You may wish to increase the resolution for $p \in [0.4, 0.7]$.) For each $p \in P$, draw N samples of a 20×20 grid with vacancy probability p. For each sample, calculate whether the grid percolates or not; the fraction of grids that percolates is our estimate for $C(p)$. Plot $C(p)$ as a function of p.

[Hint: you will need to choose suitable N and P so that the interpolation error and statistical error due to sampling are acceptable. The curve should appear smooth; if it is not, try increasing N and/or refining P.]

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Here efficiency of the code matters (for you more than for me): with a reasonable implementation, it took my code about 7 minutes to answer this question. If your implementation is very inefficient, then that could become hours, or days.

Conclusion

Best of luck with the projects!