

Introduction to Python

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Physical Methods of Biology

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How programming languages got their names



Bash

Bash is an acronym for Bourne-again Shell, a pun on the Bourne Shell - named after creator Stephen Bourne - being "born again". 'Bash' is also a verb meaning 'to strike with a heavy blow', possibly from the Danish 'baske' meaning 'to beat, strike'.



Elixir

The word 'elixir', meaning a potion or essence that prolongs life or preserves something, stems from the Arabic 'al-iks' via the late Greek 'xerion', a powder for drying wounds. Appeared in Middle English from the 14th century.



JavaScript

Originally named Mocha, a type of fine quality coffee, it was later renamed JavaScript, combining Java, US slang for coffee, + 'Script', 'something that is written' from the Latin 'scriptum', 'a set of written words or writing'.



PHP

Originally known as Personal Home Page Construction Kit, this was later shortened to just PHP (an acronym for Personal Home Page). It is now accepted as the initials for PHP: Hypertext Preprocessor.



Ruby

Influenced by Perl, the developer chose a colleague's birthstone which followed it in the monthly sequence (June is Pearl, Ruby is July). Ruby comes from the Old French 'rubi', a 'reddish precious stone', and the Latin 'rubeus', 'red'.



SQL

First called "Structured English Query Language" (SEQUEL), pronounced "sequel", it was a pun that it was the sequel to QUEL. It was later shortened to SQL. The word 'sequel' stems from the Latin 'sequela' from 'sequi' meaning 'to follow'.



C

Quite simply C got its name because it was preceded by a programming language called B. C spawned its own children including C++ and C#. It is the third letter in the English alphabet and was originally identical to the Greek letter 'Gamma'.



Go

One of the Google developers said the name Go, sometime referred to as Golang, was chosen because it was 'short and easy to type'. The word 'go', meaning 'to travel or go somewhere' stems from the Old High German 'gān' (to go).



Kotlin

Inspired by Java, it was named after Kotlin Island in Russia. Originally called Kettusaari by the Finns ('fox island') and Ketlingen by the Swedes, (maybe stemming from 'kettel' meaning 'cauldron'). After Russia won control of the island in 1703 it was renamed 'Kotling' then 'Kotlin'.



Python

Creator Guido van Rossum named Python after TV comedy Monty Python's Flying Circus. The word 'python' comes from the ancient Greek 'Puthón', the name of a huge serpent killed by the god Apollo. Later adopted as a generic term for non-poisonous snakes that constrict their prey.



Rust

Rust's name comes from a fungus that is robust, distributed, and parallel. It is also a substring of robust. Rust, also the reddish coating formed on oxidized metal, stems from the German 'rost' and possibly the Indo-European base of 'red'.



Swift

The word 'swift' means 'moving with great speed or velocity' and can be traced back to the prehistoric 'swipt' meaning 'to move in a sweeping manner'. The swallow-like bird became known as a swift from the 17th century and is used as the language's logo.



Clojure

The creator wanted to include the letter 'c' (C#), 'l' (Lisp) and 'j' (Java) and liked that it was a pun on 'closure'. The word 'closure', the act of closing, comes from the Latin 'clausura' stemming from 'claudere' which means 'to shut or close'.



Java

The name Java was the result of a highly-caffeinated brainstorming session. Java, or 'Jawa' in Indonesian, is the name of a large island in Indonesia that produces strong, dark and sweet coffee. It has been a slang term for coffee in the United States since the 1800s.



Perl

Initially named Pearl, the alternative spelling was adopted as the name was already taken. It comes from the Middle French 'perle' meaning 'bead' or 'something valuable' and the Latin 'perna' meaning 'leg', also a mollusc shaped like a leg of mutton.



R

R is named partly after the first names of the first two R authors (Ross Ihaka and Robert Gentleman) and partly as a play on the name of S, its parent language. It is the 18th letter in the alphabet and derives from the Greek letter 'Rho'.



Scala

Scala is a combination of the first letters of 'scalable' and 'language'. It is also the Italian word for 'stairway', as it helps users to ascend to a better language. The logo is also an abstraction of a staircase or steps.



TypeScript

Originating from the shortcomings of JavaScript, hence the similarity of the name. Its name combines 'Type', meaning a kind or class (from the Greek 'tuptein' 'to strike'), with 'Script', 'something that is written' from the Latin 'scriptum'.

7 REASONS

WHY PYTHON IS POPULAR WITH DEVELOPERS



Flexisource IT
Your handpicked dedicated IT team.

- ❑ Easy to Learn and Use
- ❑ Open Source with Vibrant Community
- ❑ Hundred of Pythons and Frameworks Available Online
- ❑ Supports multiple programming paradigms
- ❑ Versatile and Reliable
- ❑ Compatible with Major Platforms and Systems
- ❑ Growing Market Demand



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Example 1

Binomial distribution

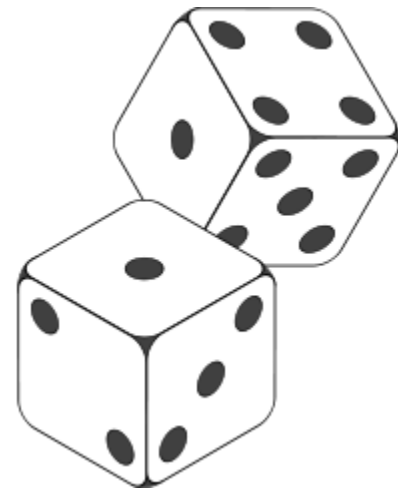
Problem: sample random numbers from a binomial distribution and compare with distribution function. Show that for $N \rightarrow \infty$ the binomial distribution tends to a Gaussian distribution.

$$B(N, n; p) = \frac{N!}{n! (N - n)!} p^n (1 - p)^{N-n} \rightarrow \mathcal{N}(Np, Np(1 - p))$$

Example 2

Rolling a die

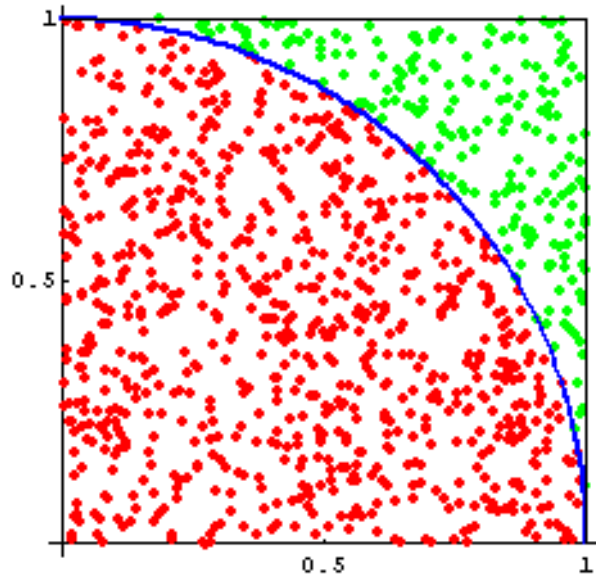
Problem: simulate N rolls of a die. Show the evolution of the histogram of extracted values at each roll. Check that for $N \rightarrow \infty$ the probability of finding each face is $1/6$. Simulate an unfair die.



Example 3

Monte Carlo

Problem: calculate π using the Monte Carlo integration method. How many iterations are needed to get 10 significant digits of π ?

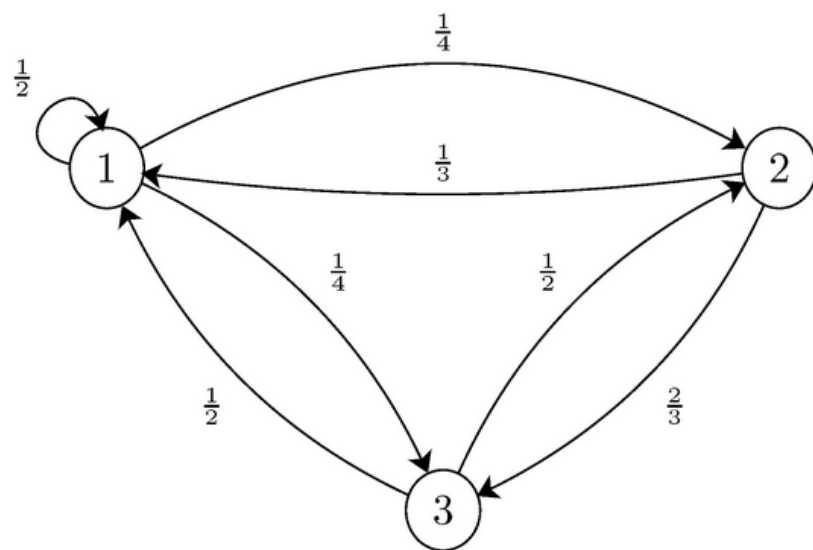


$$\frac{N_{in}}{N_{in} + N_{out}} \rightarrow \frac{\pi}{4}$$

Example 4

Markov Chains

Problem: consider the Markov chain shown in the diagram. Simulate the trajectory of one particle starting from initial state 1. Simulate the trajectories of N particles (starting from randomly assigned initial states) and check that the probability distribution tends to the equilibrium state..



$$\pi = \begin{pmatrix} 1/2 & 1/3 & 1/2 \\ 1/4 & 0 & 1/2 \\ 1/4 & 2/3 & 0 \end{pmatrix}$$

$$\rho_{\text{eq}} = \begin{pmatrix} 0.457 \\ 0.257 \\ 0.286 \end{pmatrix}$$

Example 5

Monty Hall

Problem: give a numerical solution of the Monty Hall problem.

Monty Hall problem.

Suppose you're on a game show, and you're given the choice of three doors.

Behind one door is a car; behind the others, goats.

You pick a door, say No. 1, and the host, who knows what's behind the doors, opens another door, say No. 3, which has a goat.

He then says to you, "Do you want to pick door No. 2?"

Is it to your advantage to switch your choice?



Exam projects

My project

Hydrogen Deuterium Exchange Mass Spectrometry (HDX-MS)

Re-implement and reproduce the results of a recently published paper about a novel method to analyse HDX-MS data and estimate the “protection factors” of a protein.

Biophysical *Journal*
Article



Estimating Constraints for Protection Factors from HDX-MS Data

Simon P. Skinner,^{1,2} Gael Radou,^{1,2} Roman Tuma,^{1,2,3} Jeanine J. Houwing-Duistermaat,^{4,5}
and Emanuele Paci^{1,2,*}

¹Astbury Centre for Structural Molecular Biology and ²School of Cellular and Molecular Biology, University of Leeds, Leeds, United Kingdom;
³Faculty of Science, University of South Bohemia, České Budějovice, Czech Republic; ⁴School of Mathematics, University of Leeds, Leeds,
United Kingdom; and ⁵Department of Biostatistics and Research Support, Julius Center, UMC Utrecht, The Netherlands

Exam projects

My project → a (small) paper

Hydrogen Deuterium Exchange Mass Spectrometry (HDX-MS)

Re-implement and reproduce the results of a recently published paper about a novel method to analyse HDX-MS data and estimate the “protection factors” of a protein.

Find and analyse a dataset probing the same protein (mouse prion protein) with HDX-MS and a complementary experiment (HDX-NMR) to validate the method.
Are the “protection factors” estimated from the two experiments compatible?

ACS Partner Journal



Journal of the American Society for
Mass Spectrometry



pubs.acs.org/jasms

Research Article

High-Resolution Hydrogen–Deuterium Protection Factors from Sparse Mass Spectrometry Data Validated by Nuclear Magnetic Resonance Measurements

Michele Stofella, Simon P. Skinner, Frank Sobott, Jeanine Houwing-Duistermaat, and Emanuele Paci*

Exam projects

My project → a (small) paper → my thesis

Hydrogen Deuterium Exchange Mass Spectrometry (HDX-MS)

Re-implement and reproduce the results of a recently published paper about a novel method to analyse HDX-MS data and estimate the “protection factors” of a protein.

Find and analyse a dataset probing the same protein (mouse prion protein) with HDX-MS and a complementary experiment (HDX-NMR) to validate the method.
Are the “protection factors” estimated from the two experiments compatible?

Develop a previously published microscopic model which aims to calculate “protection factors” from MD simulations. The model is a function of two variables (number of hydrogen bonds and number of heavy contacts); I tried to insert a dependence on local electrostatic properties.

The work was boosted by a 4-month Erasmus+ internship at the University of Leeds.

ALMA MATER STUDIORUM · UNIVERSITY OF BOLOGNA	
School of Science Department of Physics and Astronomy Master Degree in Physics	
Hydrogen Deuterium Exchange: Methods to Probe Protein Dynamics at Single Residue Resolution	
Supervisor: Prof. Gastone Castellani	Submitted by: Michele Stofella
Co-supervisor: Prof. Emanuele Paci	
Academic Year 2019/2020	

Exam projects

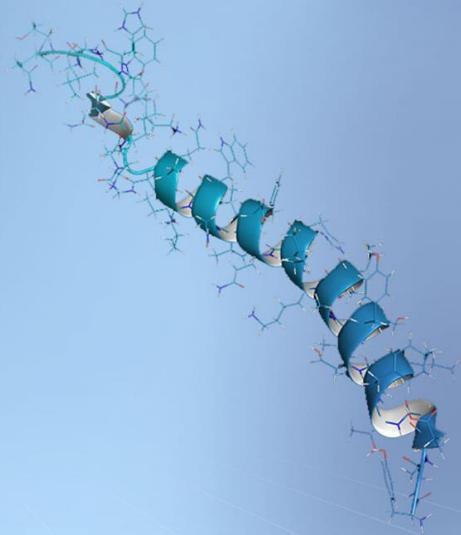
Some ideas

Polymer Physics

Homopolypeptides

(from Boulger dissertation)

Proteins are polymers composed of amino acids. Analysis of all available protein structures and molecular dynamics simulations show that secondary structural propensity of proteins depends on the chain length. Simple sequences such as homopolypeptides have shown protein-like secondary structure and a continuous transition between mostly alpha-helical to a beta-sheet-rich compact conformation as the length of the chain increases. This is observed for some homopolypeptides, the critical length for a propensity change from mainly alpha to mainly beta conformation varies with each amino acid, for polythreonine and polyvaline the intrinsic propensity transition is observed beyond a chain length of 25 amino acids and 15 amino acids respectively. Analysis of structures in the protein data bank also shows a reassuring agreement with the simulation results.



Exam projects

Some ideas

Protein Dynamics

Interactive Molecular Dynamics in Virtual Reality

Interactive Molecular Dynamics in Virtual Reality Is an Effective Tool for Flexible Substrate and Inhibitor Docking to the SARS-CoV-2 Main Protease

Helen M. Deeks,[†] Rebecca K. Walters,[†] Jonathan Barnoud, David R. Glowacki,^{*} and Adrian J. Mulholland^{*}

Training Neural Nets To Learn Reactive Potential Energy Surfaces Using Interactive Quantum Chemistry in Virtual Reality

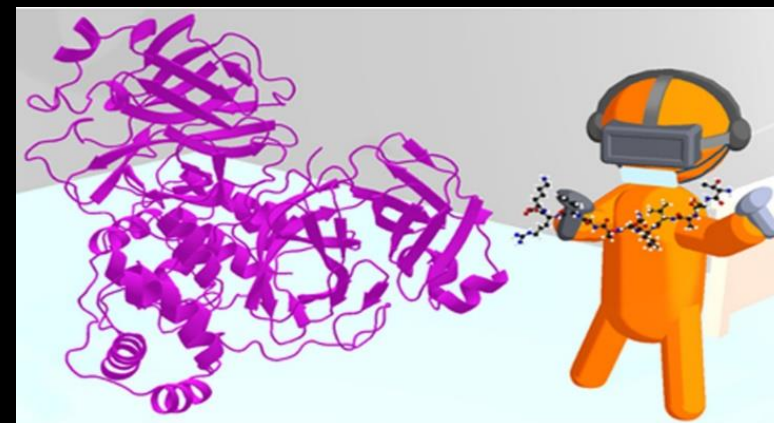
Published as part of The Journal of Physical Chemistry virtual special issue "Young Scientists".

Silvia Amabilino,^{†,‡,⊥} Lars A. Bratholm,^{†,‡,⊥} Simon J. Bennie,^{†,‡} Alain C. Vaucher,[§] Markus Reiher,[§] and David R. Glowacki^{*,†,‡,⊥}

[†]School of Chemistry, University of Bristol, Bristol BS8 1TS, U.K.

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Exam projects

Some ideas

Didactics of Physics

Molecular Dynamics in Virtual Reality

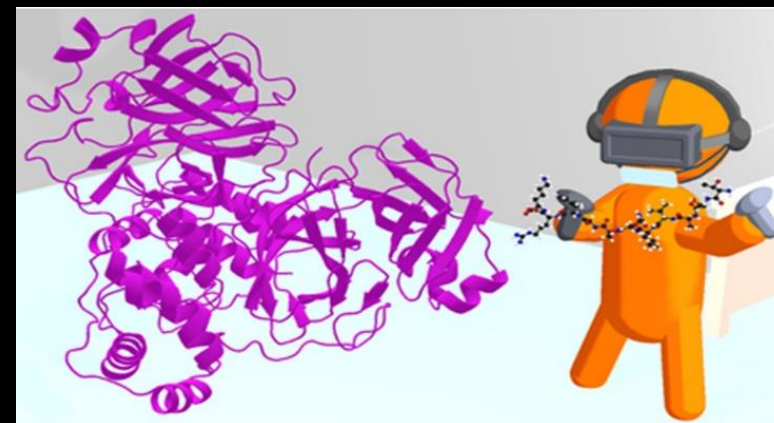
Teaching Enzyme Catalysis Using Interactive Molecular Dynamics in Virtual Reality

Simon J. Bennie,^{*,†,‡,§} Kara E. Ranaghan,^{†,§} Helen Deeks,^{†,‡,§} Heather E. Goldsmith,
Michael B. O'Connor,^{†,‡,§} Adrian J. Mulholland,^{*,†,§} and David R. Glowacki^{*,†,‡,§}

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Exam projects

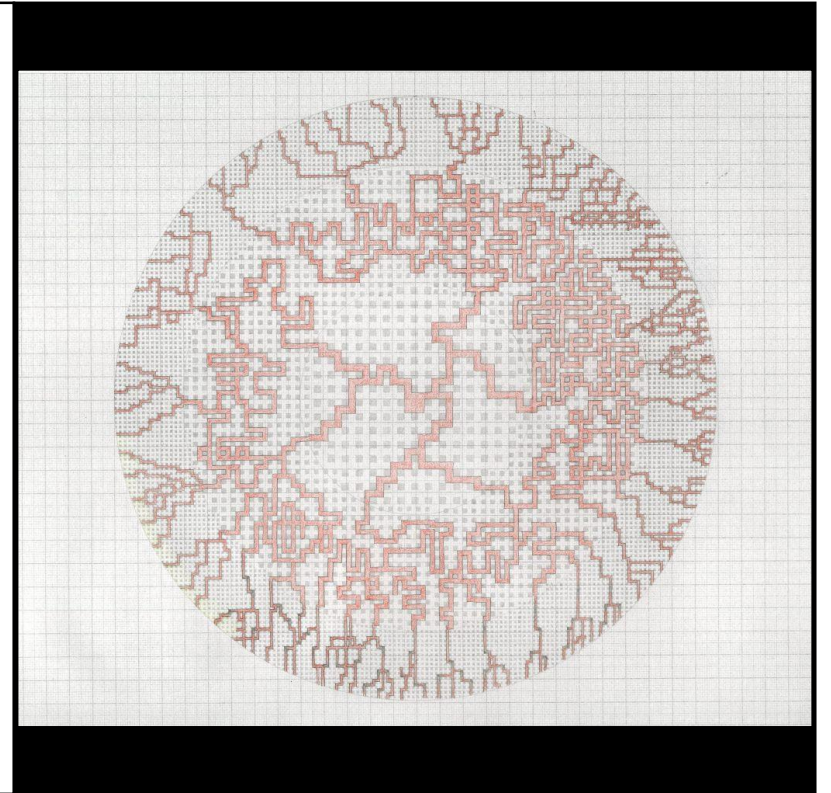
Some ideas

Didactics of Physics

Teaching and visualizing protein folding

(from <https://www.gemma-anderson.co.uk/image/maze-energetics-of-a-protein/>)

Proteins pervade life and collectively they take an infinite variety of forms. Protein's fold, most of the time this is what a protein is trying to do. The folded protein is the relaxed protein, in its 'natural' state, not wasting any energy. Folding is a process, it happens through time, in an 'energy landscape' often imagined to be conical (cone shaped) with the folded protein resting in the very bottom – the point of least energy in the landscape. As the protein moves from the top of this landscape to the bottom (it might not make it) it embarks on an explorative journey of the space; body and environment continuously co-creating each other. There are fast and slow tracks, uphill and downhill, dead-ends and if in trouble then a 'chaperone' will come to help find the way together. This dynamic process is hard to imagine and the images you find in scientific textbooks don't exactly give the game away (generally a cone, a few uphill or downhill). How else can we imagine this complexity? What other images could we see?



Feel free to contact me for questions/opinions:

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