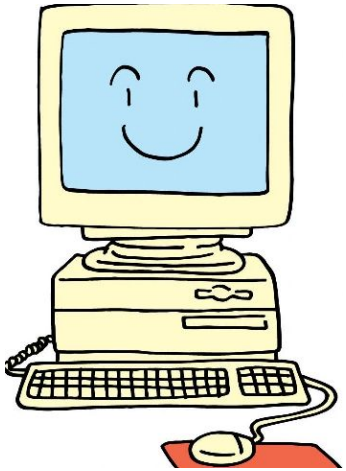
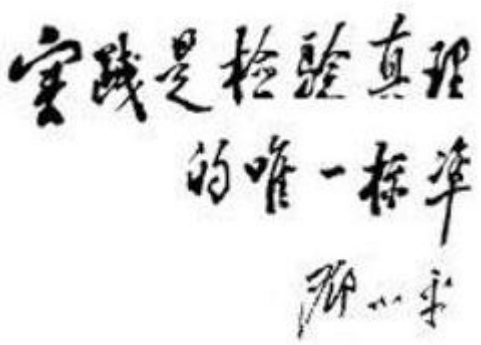
计算物理 第一部分
第1讲





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五次大作业，最终成绩是5次作业成绩的平均，占总成绩的70%。**期末闭卷考试，占总成绩的30%。**

这些作业中，有相当的内容是同学们利用所学的算法自己编写程序解决一些具体的数学或物理问题，你们**需要附上源代码以及数值结果，加上对结果的分析和讨论**。严禁从任何渠道抄袭（包括网上、书籍或(往届)同学等），**一旦发现一次，该次作业成绩为0；发现二次及以上，平时作业为0。**

本课程不讲授具体高级程序设计语言，默认选课同学已掌握或者将自学至少下面一种高级语言：Fortran, C, C++或者Python等。**我们不接受利用Mathematica或者Matlab等集成软件，或者调用Python库编写的程序完成作业！**

每次作业会安排抽查，由助教约谈几位同学，要求同学当场演示讲解。

- **计算物理**，是利用计算机来求解物理问题或者分析物理实验结果的一个重要的物理学分支，有其相对的独立性；同时，它是**物理学、数学、计算机科学三者的交叉学科**，与理论物理和实验物理有着密切的联系，为物理学的发展起着极大的推动作用。
  现代科学分析三大手段之一：理论分析、科学实验、数值计算。

- 计算物理的**研究目标是物理**，**但其核心是数值分析，也称为数值计算(或科学计算)**。在数学科学里，数值分析也叫计算数学，是数学科学的一个重要分支，其研究对象是利用计算机求解各种数学问题的数值方法及相关理论。

- **数值计算和分析**在众多的学科和应用中占有举足轻重的地位，几乎涉及到自然科学、工程应用和社会科学的各方面。

大型科学计算的发展水平也是一个国家综合国力的重要标志之一(硬件+软件)： http://www.top500.org **(全球超算500)**

无论是国防、材料科学、天文学，还是距离我们生活更近的天气预报、灾害监测、交通管理，超算都大有用武之地。中国「天河二号」超算协助搭建起「15秒断诊」的新冠CT影像智能诊断平台，并助力筛选能抑制病毒的小分子药物。美国Summit超算同样参与到新药研制中，模拟新冠病毒与不同化合物的反应。2020/2021夺冠的日本Fugaku超算也为探索新药启动了试验。
https://www.top500.org/lists/top500/2022/06/

Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
1	**Frontier** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE DOE/SC/Oak Ridge National Laboratory United States	8,730,112	1,102.00	1,685.65	21,100
2	**Supercomputer Fugaku** - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442.01		
3	**LUMI** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE EuroHPC/CSC Finland	1,110,144	151.90		

Computer performance

Name	Unit	Value
kiloFLOPS	kFLOPS	10^3
megaFLOPS	MFLOPS	10^6
gigaFLOPS	GFLOPS	10^9
teraFLOPS	TFLOPS	10^{12}
petaFLOPS	PFLOPS	10^{15}
exaFLOPS	EFLOPS	10^{18}

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以前传统是三种手段

一个是理论推导

二是物理实验 实验验证

三是基于计算机做模拟计算

现在又多了一种手段是

大数据分析

数值计算方法的历史：

- 有不少计算方法是非常传统的，它们在18-19世纪或者更早些时候就已经建立。**20世纪40年代电子计算机的问世及之后的飞速发展**，为大规模的数值计算创造了条件，也使得集中而系统的研究适用于数字计算机的数值算法变得十分迫切和必要。
- 数值分析作为一门学科分支，不仅仅是一些数值方法的简单积累，而**需要揭示包含在多种数值方法之间的相同结构和统一的原理**。它在大量数值计算实践和理论分析工作的相互促进中迅速发展着。有些原有方法沿用至今，有一些被淘汰，而新的方法和理论不断诞生。

- 数值计算的早期历史：

  H. H. Goldstine. *A history of Numerical Analysis from the 16th through the 19th Century*. Springer-Verlag, New York, 1977.

- 科学计算在计算机时代的历史：

  S. G. Nash, editor. *A History of Scientific Computing. ACM Press*, New York, 1990.

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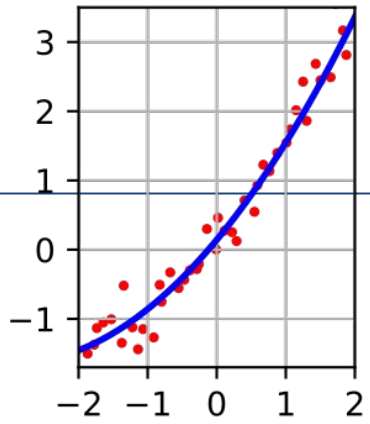


Colin Maclaurin

Drawing by David Steuart Erskine c. 1795, from a portrait by James Ferguson

Born	February 1698 Kilmodan, Cowal, Argyll, Scotland
Died	14 June 1746 (aged 48) Edinburgh, Scotland

Leonhard Euler

Portrait by Jakob Emanuel Handmann (1753)

Born	15 April 1707 Basel, Switzerland
Died	18 September 1783 (aged 76)

Joseph-Louis Lagrange

Joseph-Louis (Giuseppe Luigi), comte de Lagrange

Born	Giuseppe Lodovico Lagrangia 25 January 1736 Turin, Kingdom of Sardinia
Died	10 April 1813 (aged 77) Paris, First French Empire

Pierre-Simon Laplace

Pierre-Simon Laplace as Chancellor of the Senate under the First French Empire

Born	23 March 1749 Beaumont-en-Auge, Normandy, Kingdom of France
Died	5 March 1827 (aged 77) Paris, Kingdom of France

Adrien-Marie Legendre

1820 watercolor caricature of Adrien-Marie Legendre by French artist Julien-Léopold Boilly (see mistaken portrait), the only existing portrait known[1]

Born	18 September 1752 Paris, France
Died	9 January 1833 (aged 80) Paris, France

Carl Friedrich Gauss

Portrait of Gauss by Christian Albrecht Jensen (1840)

Born	Johann Carl Friedrich Gauss 30 April 1777 Brunswick, Principality of Brunswick-Wolfenbüttel
Died	23 February 1855 (aged 77)

Augustin-Louis Cauchy

Cauchy around 1840. Lithography by Zéphirin Belliard after a painting by Jean Roller.

Born	21 August 1789 Paris, France
Died	23 May 1857 (aged 67) Sceaux, France

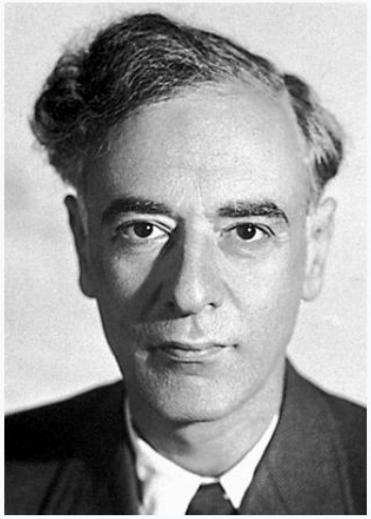
Carl Gustav Jacob Jacobi

Born	10 December 1804 Potsdam, Kingdom of Prussia
Died	18 February 1851 (aged 46) Berlin, Kingdom of Prussia

朗道《力学》：“理论物理的目标是建立物理定律，即建立物理量之间的关系。**确定物理量的具体数值一般不是理论物理的任务，实验在处理这些问题方面相对比较容易**，因为在绝大多数情况下，实验不必进行花费大量时间和人力的计算。当然，用理论可以直接算出数值的简单的情况除外”。在朗道看来，从理论出发算出数值的结果是很困难，朗道之所以有这样的论断是因为他写《力学》这本书的时候是在上世纪中叶，**那时的计算手段很落后，数值计算比实验还要困难。**但我们今天借助庞大的计算机，可以做很多前人想都无法想象的事情。

这门课如果是数学系开可能会被称为**Numerical analysis**，如果是计算机系开，可能会被称为**Numerical computing**，我们物理学院开，称之为**计算物理**。事实上，**随着计算机技术的发展，计算物理是作为实验物理、理论物理之外的第三大分支存在的。**它的作用是让我们通过数值的方法去解决我们在科研、工程中所遇到的各种物理问题。**这与我们学院开的另外一门课，数学物理方法正好相辅相成。**数理方法是要通过解析的手段去解决物理问题。

Lev Landau



Born	Lev Davidovich Landau 22 January 1908 Baku, Baku Governorate, Russian Empire
Died	1 April 1968 (aged 60) Moscow, Soviet Union

众所周知，物理学是由实验物理和理论物理两个学科组成的.我们已知的大量物理定律可以由为数不多的最一般规律推演出来.这样的推演和最一般规律的建立需要独特的方法，这些构成了特别的学科——理论物理学的任务.

理论物理利用数学手段和方法得出自己的结果和结论，但理论物理与数学的截然不同在于前者与实验结果的直接联系，且不说最一般规律的建立只能以实验数据为基础，甚至从一般规律中得到推论也需要对现象做预先的实验研究，没有这样的实验研究，就无法从大量参与因素中判断哪些因素是重要的，哪些因素是可以忽略的.在得到只考虑重要因素的方程之后，从本质上说，理论物理的任务就基本完成了.进一步应用这些方程于复杂程度不同的具体情况很快成为数学的研究对象，由称为数学物理的一个数学分支来研究.

理论物理的目标是建立物理定律，即建立物理量之间的关系.确定物理量的具体数值一般不是理论物理的任务，实验在处理这些问题方面相对比较容易，因为在绝大多数情况下，实验不必进行花费大量时间和人力的类似的计算.当然，用理论可以直接算出数值的简单情况除外①.

必须指出，由于理论物理的任务是建立刻画给定现象的物理量之间的联系，因此只有在自然界确实存在这种联系时，才能建立理论.但是，经常是我们感兴趣的物理量之间毫无关系，亦即在不同的自然现象中可以在极为不同的组合中遇到这些物理量.因此，缺乏某个现象的理论并不意味着它无法解释.如同在其它情况下规律性可以由最一般的规律得出一样，在这种情况下不存在规律性的

① 朗道写这个序言是在1940年，那时的计算手段很落后，所以数值计算比实验还困难.——译者注

研制原子弹时也使用更酷的手摇计算机

手摇计算机是1878年由一位在俄国工作的瑞典发明家奥涅尔制造的。
手摇计算机一般只能做四则运算、平方数、立方数、开平方、开立方。如果需要输入三角函数和对数，都需要查表。如果计算中有括号，麻烦极了。使用中必须正摇几圈，反摇几圈，还要用纸笔不断记录。

数值计算于国防：氢弹之父于敏

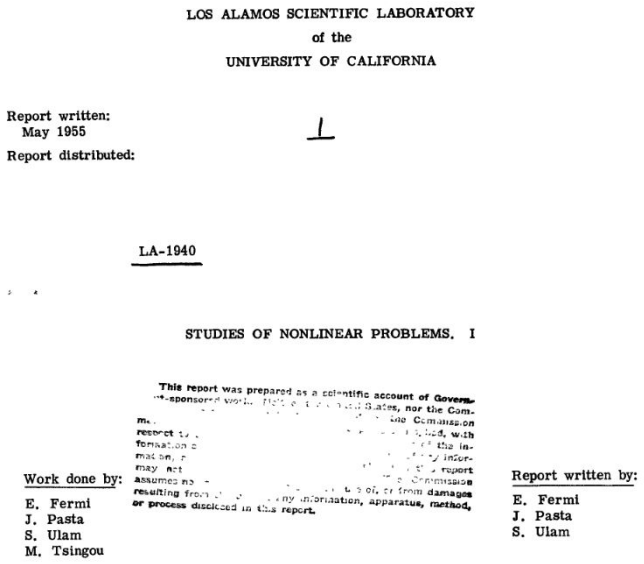
【校友撷英】于敏：民族的脊梁北大人的榜样：
“而国内当时(1965年左右)仅有一台每秒万次的电子管计算机，并且95%的时间分配给有关原子弹的研究，只剩下5%的时间留给于敏负责的氢弹设计。”

计算机最初是为开发核武器以及破译密码之用的,但在 20 世纪 50 年代初期就部分转为非军事用途,特别是 Metropolis 等人在计算机上尝试尽可能广泛的不同问题,以评价其逻辑结构及证实其能力。

在 E. Fermi 的推动下,1952 年起洛斯阿拉莫斯实验室开始将计算机应用于非线性系统的长时间行为和大尺度性质的研究。
1955 年 5 月由 Fermi 等编写的洛斯阿拉莫斯实验室报告中提出了许多重要物理问题,被许多人看成是计算物理的正式起点。

https://www.osti.gov/servlets/purl/4376203
https://pubs.aip.org/physicstoday/article/61/1/55/413049/Fermi-Pasta-Ulam-and-a-mysterious-ladyThe

Studies of Nonlinear Problems



LOS ALAMOS SCIENTIFIC LABORATORY
of the
UNIVERSITY OF CALIFORNIA

Report written:
May 1955

Report distributed:

1

LA-1940

STUDIES OF NONLINEAR PROBLEMS. I

This report was prepared as a scientific account of Govern-
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or process disclosed in this report.

Work done by:
E. Fermi
J. Pasta
S. Ulam
M. Tsingou

Report written by:
E. Fermi
J. Pasta
S. Ulam

A one-dimensional dynamical system of 64 particles with forces between neighbors containing nonlinear terms has been studied on the Los Alamos computer **MANIAC** I. The nonlinear terms considered are quadratic, cubic, and broken linear types. The results are analyzed into Fourier components and plotted as a function of time. The results show very little, if any, tendency toward equipartition of energy among the degrees of freedom.

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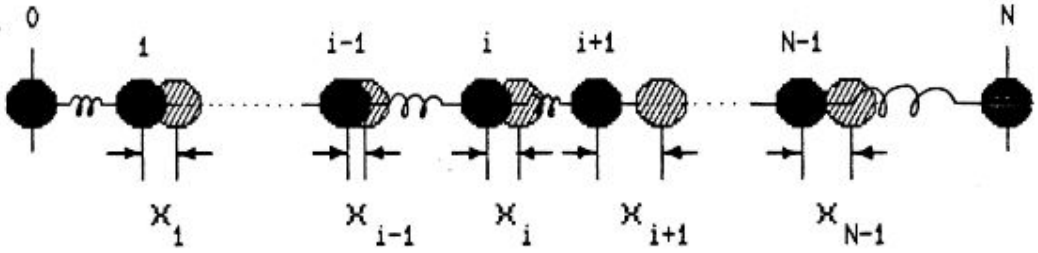
* We thank Miss Mary Tsingou for efficient coding of the problems and for running the computations on the Los Alamos MANIAC machine.

The last few examples were calculated in 1955. After the untimely death of Professor E. Fermi in November, 1954, the calculations were continued in Los Alamos.

https://pubs.aip.org/physicstoday/article/61/1/55/413049/Fermi-Pasta-Ulam-and-a-mysterious-ladyThe
Physics Today ***61*** *(1), 55–57 (2008);*

The Fermi-Pasta-Ulam (FPU) problem, first written up in a Los Alamos report in May 1955, **marked the beginning of both a new field, nonlinear physics, and the age of computer simulations of scientific problems**. The idea was to simulate the one-dimensional analogue of atoms in a crystal: **a long chain of masses linked by springs that obey Hooke's law** (a linear interaction), **but with a weak nonlinear term**. A purely linear interaction would ensure that energy introduced into a single Fourier vibrational mode always remains in that mode; **the nonlinear term allows the transfer of energy between modes**. Under certain conditions, **the weakly nonlinear system exhibits surprising behavior: The energy does not drift toward the equipartition predicted by statistical physics but periodically returns to the original mode**. That highly remarkable result, known as the FPU paradox, shows that nonlinearity is not enough to guarantee the equipartition of energy.



$$x_i = (x_{i+1} + x_{i-1} - 2x_i) + \alpha\left[(x_{i+1} - x_i)^2 - (x_i - x_{i-1})^2\right]$$

$$i = 1, 2, \ldots 64,$$

or

$$x_i = (x_{i+1} + x_{i-1} - 2x_i) + \beta\left[(x_{i+1} - x_i)^3 - (x_i - x_{i-1})^3\right]$$

$$i = 1, 2, \ldots 64.$$

https://icsabai.github.io/simulationsMsc/ProjectFPU.pdf

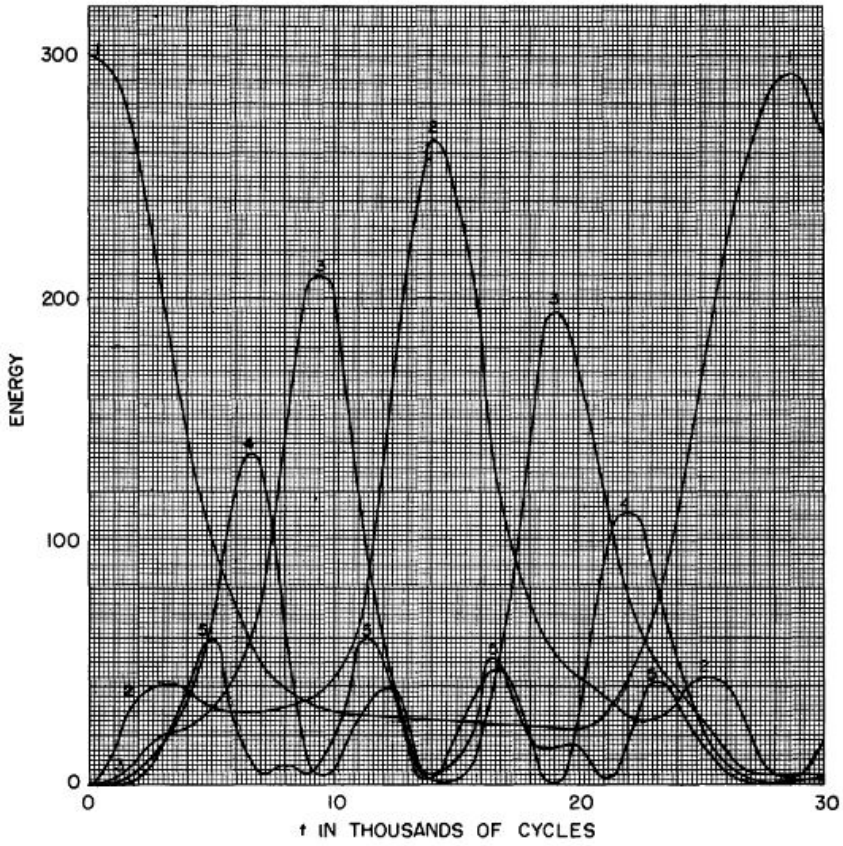
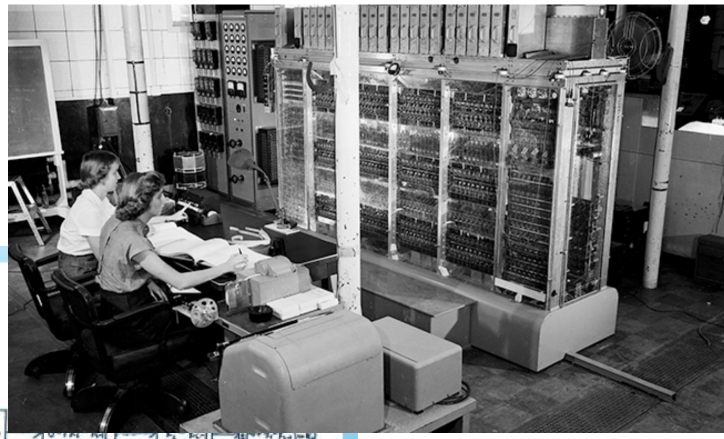
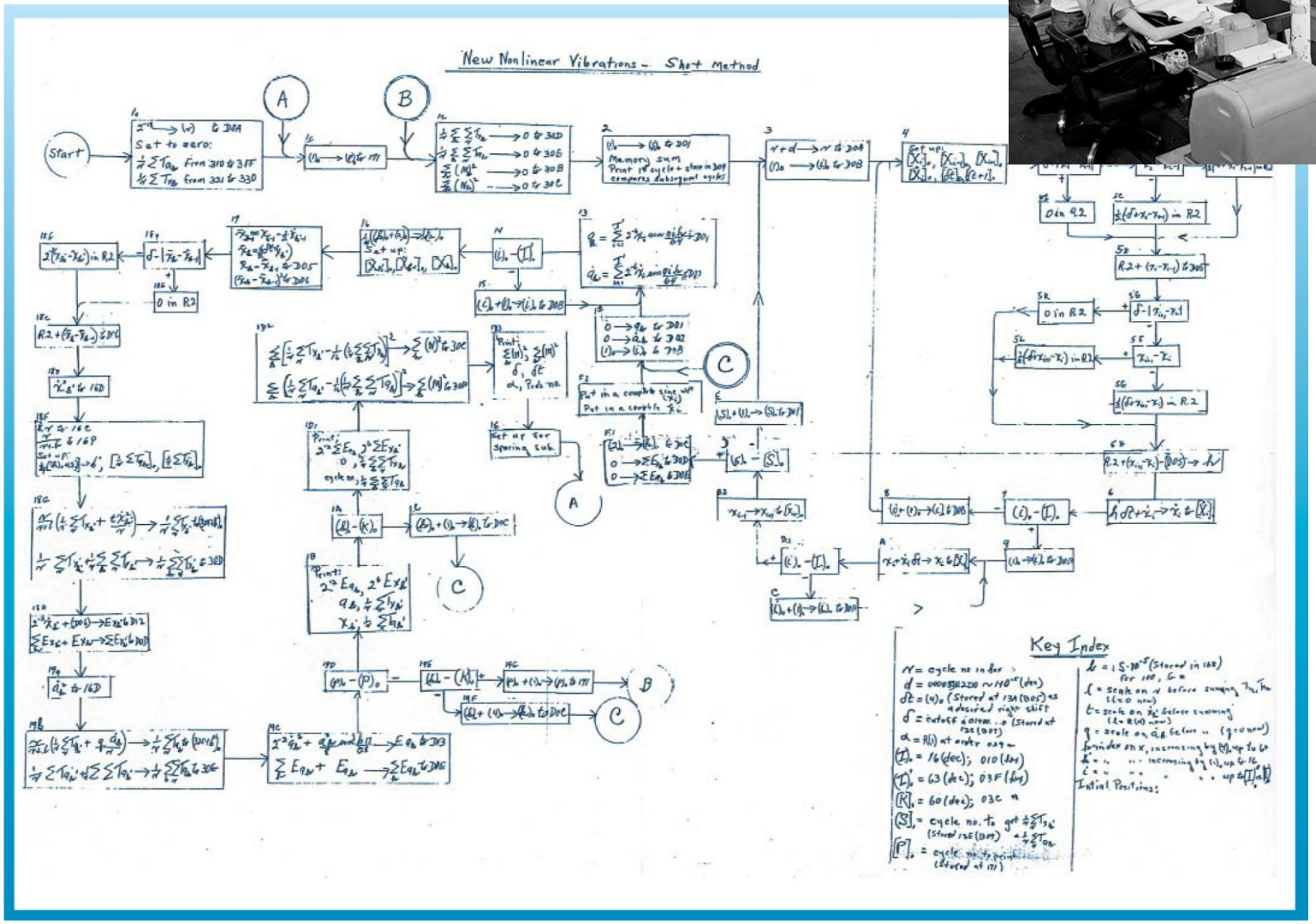


Fig. 1. The quantity plotted is the energy (kinetic plus potential in each of the first five modes). The units for energy are arbitrary. $N = 32$; $\alpha = 1/4$; $\delta t^2 = 1/8$. The initial form of the string was a single sine wave. The higher modes never exceeded in energy 20 of our units. About 30,000 computation cycles were calculated.

https://pubs.aip.org/physicstoday/article/61/1/55/413049/Fermi-Pasta-Ulam-and-a-mysterious-ladyThe





Fermi, Pasta, Ulam and the Birth of Experimental Mathematics

A numerical experiment that Enrico Fermi, John Pasta, and Stanislaw Ulam reported 54 years ago continues to inspire discovery

Mason A. Porter, Norman J. Zabusky, Bambi Hu and David K. Campbell

Four years ago, scientists around the globe commemorated the centennial of Albert Einstein's 1905 *annus mirabilis*, in which he published stunning work on the photoelectric effect, Brownian motion and special relativity—thus reshaping the face of physics in one grand swoop. Intriguingly, 2005 also marked another important anniversary for physics, although it passed unnoticed by the public at large. Fifty years earlier, in May 1955, Los Alamos Scientific Laboratory (as it was then known) released technical report LA-1940, titled "Studies of Nonlinear Problems: I." Authored by Enrico Fermi, John Pasta and Stanislaw Ulam, the results presented in this document have since rocked the scientific world. Indeed, it is not an exaggeration to say that the FPU problem, as the system Fermi, Pasta and Ulam studied is now universally called, sparked a revolution in modern science.

Time After Time

In his introduction to the version of LA-1940 that was reprinted in Fermi's collected works in 1965, Ulam wrote that Fermi had long been fascinated by a fundamental mystery of statistical mechanics that physicists call the "arrow of time." Imagine filming the collision of two billiard balls: They roll toward each other, collide, and shoot off in other directions. Now run your film backwards. The motion of the balls looks perfectly natural—and why not: Newton's laws, the equations that govern the motion of the balls, work equally well for both positive and negative times.

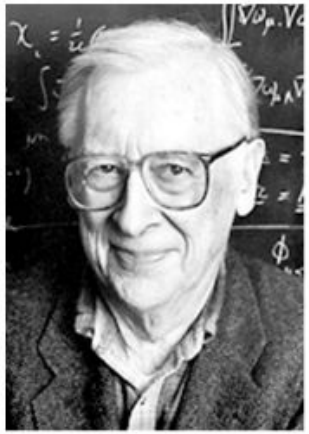
Now imagine the beginning of a game of billiards—actually, American

tunately, because he was at Los Alamos in the early 1950s, he had access to one of the earliest digital computers. The Los Alamos scientists playfully called it the MANIAC (MAthematical Numerical Integrator And Computer). It performed brute-force numerical computations, allowing scientists to solve problems (mostly ones involving classified research on nuclear weapons) that were otherwise inaccessible to analysis. The FPU problem was one of the first open scientific investigations carried out with the MANIAC, and it ushered in the age of what is sometimes called experimental mathematics.

The phrase "experimental mathematics" might seem like an oxymoron: Everyone knows that the validity of mathematics is independent of what goes on in the physical world. Nev-

数值计算于科研：1998和2013年诺贝尔化学奖


Walter Kohn


John A. Pople


Martin Karplus


Michael Levitt

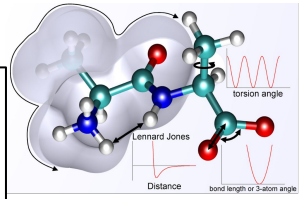

Arieh Warshel

Walter Kohn "for his development of the density-functional theory" and John A. Pople "for his development of computational methods in quantum chemistry".

"for the development of multiscale models for complex chemical systems".

这三位都是分子模拟的开山鼻祖，他们开创的领域广泛应用于化学、材料、生物，终于在30多年后获得了诺贝尔奖

Kohn 在大学和硕士研究生阶段是学习应用数学的,在博士研究生时期跟随著名理论物理学家 Schwinger 转攻物理学,从而奠定了他的多学科的知识背景,为他在其后的计算凝聚态物理学上取得重大成就贡献打下了良好的基础



The Nobel Prize in Physics 1999

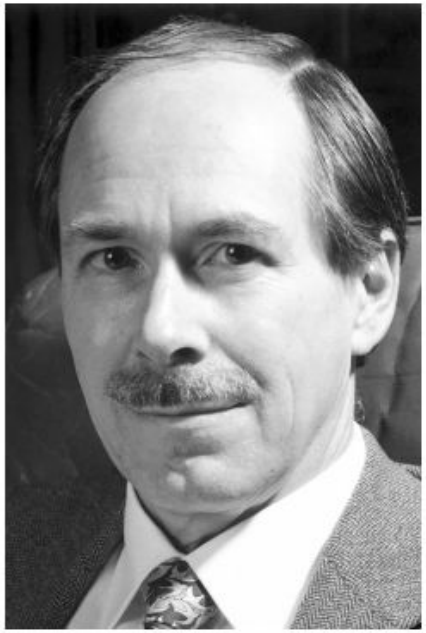


Photo from the Nobel Foundation archive.

Gerardus 't Hooft

Prize share: 1/2

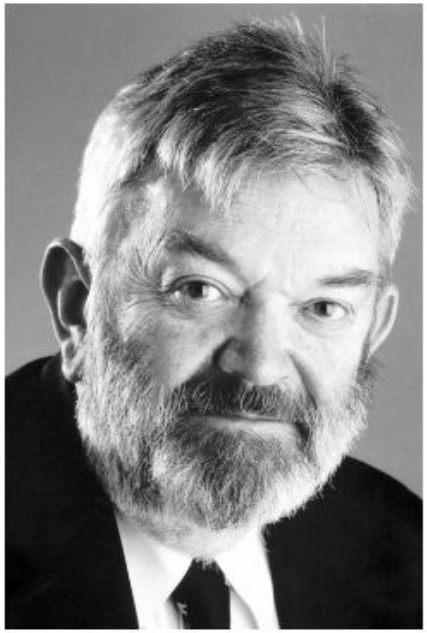


Photo from the Nobel Foundation archive.

Martinus J.G. Veltman

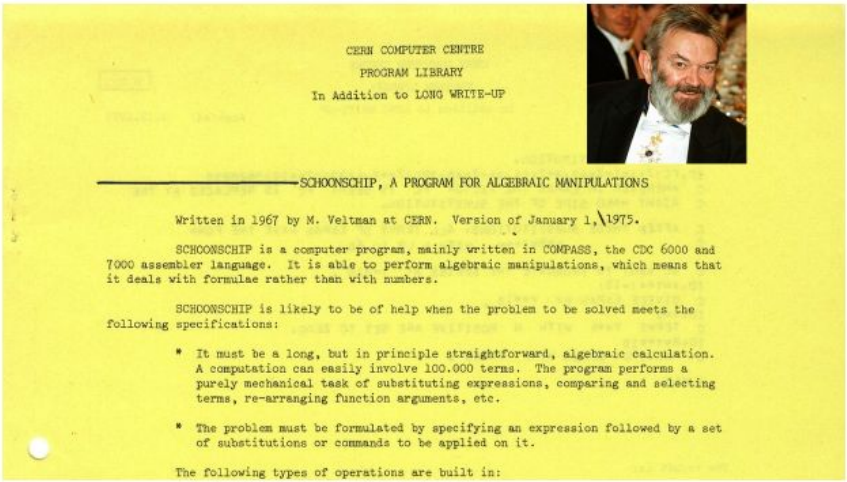
Prize share: 1/2

Tini Veltman (1931–2021): From Assembly Language to a Nobel Prize

汇编语言 符号运算

January 21, 2021

link



CERN COMPUTER CENTRE
PROGRAM LIBRARY
In Addition to LONG WRITE-UP

SCHOONSCHIP, A PROGRAM FOR ALGEBRAIC MANIPULATIONS

Written in 1967 by M. Veltman at CERN. Version of January 1, 1975.

SCHOONSCHIP is a computer program, mainly written in COMPASS, the CDC 6000 and 7000 assembler language. It is able to perform algebraic manipulations, which means that it deals with formulae rather than with numbers.

SCHOONSCHIP is likely to be of help when the problem to be solved meets the following specifications:

* It must be a long, but in principle straightforward, algebraic calculation. A computation can easily involve 100.000 terms. The program performs a purely mechanical task of substituting expressions, comparing and selecting terms, re-arranging function arguments, etc.

* The problem must be formulated by specifying an expression followed by a set of substitutions or commands to be applied on it.

The following types of operations are built in:

The Nobel Prize in Physics 1999 was awarded jointly to Gerardus 't Hooft and Martinus J.G. Veltman "for elucidating the quantum structure of electroweak interactions in physics."

Stephen Wolfram:

Within days after finishing my PhD in theoretical physics at Caltech in November 1979, I flew to Geneva, Switzerland, to visit CERN for a couple of weeks. **And it was during that visit that I started designing SMP ("Symbolic Manipulation Program")—the system that would be the forerunner of Mathematica and the Wolfram Language.** And when I mentioned what I was doing to people at CERN they said "You should talk to Tini Veltman".

Stephen Wolfram

Wolfram in 2008

Born	29 August 1959 (age 62) London, England
Nationality	British, American
Education	Dragon School[1] Eton College
Alma mater	St. John's College, Oxford (no degree) California Institute of Technology (PhD, 1980)
Known for	Mathematica

https://arxiv.org/pdf/2208.04285.pdf

"I probably first met Kip at Princeton when he was a graduate student of Johnny Wheeler and I was a post-doc-lecturer there having just completed my PhD with Murray Gell-Mann at Caltech in 1963."

Recollections of Kip Thorne

James Hartle

Department of Physics, University of California, Santa Barbara, California 93106, USA and

II. THE KIP THORNE SCHOOL OF COMPUTING

Kip had definite ideas on how to organize computing:

- Forget Runge-Kutta and just use the simplest trapezoidal rule.
- Forget optimizing for expense and spend as much as is necessary to get the job done.
- Stay up all night if you have to, but get the job done by the morning. (And Kip and I did stay up very late in the computer room at Caltech.)

"...Kip and I were using an **IBM 7094** at Caltech and a similar machine at UCSB. Input was by punched cards and output was on many sheets of large computer paper. The 7094's computing power is sometimes compared to that of a present day musical Japanese Christmas card. **We thought of a program with three hundred Fortran statements as a large program.** We published our numerical models and their implications in (J. B. Hartle and K.S. Thorne, Slowly Rotating Relativistic Stars, II. Models for Neutron and Supermassive Stars, Ap. J. 153, 807-834, (1968))."

IEEE，也就是电器与电子工程师学会主办的《Computing in science & engineering》杂志曾经选出过 20 世纪的十大算法，也就是对科学和工程发展影响最大的十个算法：

THE TOP 10 LIST

Definition:
"An algorithm is a sequence of finite computational steps that transforms an input into an output" [Cormen and Leiserson, 2009]

1946: The Metropolis Algorithm
1947: Simplex Method
1950: Krylov Subspace Method
1951: The Decompositional Approach to Matrix Computations
1957: The Fortran Optimizing Compiler
1959: QR Algorithm
1962: Quicksort
1965: Fast Fourier Transform
1977: Integer Relation Detection
1987: Fast Multipole Method

Dantzig von Neumann Hestenes Householder Backus Hoare Greengard

1. 1946 年，美国 Los Alamos 国家实验室的 John Von Neumann(冯诺伊曼)、S. Ulam、N. Metropolis开创的**Metropolis算法，也就是蒙特卡罗方法**。
2. 1947 年，美国 RAND 公司的 G. Dantzig 开创的 Simplex 算法 (解线性规划问题)
3. 1950 年，美国国家标准局数值分析研究所的 M. Hestenes、E. Stiefel 和 C. Lanczos 开创的**Krylov子空间迭代法 (例如：解稀疏矩阵本征值和本征矢量)**
4. 1951 年，美国 Oak Ridge 国家实验室的 A. Householder(豪斯霍尔德) 形式化的**矩阵计算的分解方法，也称 Householder约化**
5. 1957 年，美国 IBM 公司的 J. Backus 领导开发的 **FORTRAN 最优编译器算法**
6. 1959 - 1961 年，英国伦敦 Ferranti 公司的 J. Francis 开创的 **QR 算法，是一种计算矩阵特征值的稳定算法** (如果待求的矩阵不是特别巨大 (n≤3000)，那么 QR 算法实际上是最为合适的算法。)
7. 1962 年，英国伦敦 Elloit Brothers 公司的 T. Hoare 提出 Quicksort 算法，也即快速排序算法 (这个算法可能大家比较熟悉，从数列中挑出一个元素，比这个基准元素小的数放在基准前面，大的数放在基准后面，然后进行递归操作就行了。)
8. 1965 年，美国 IBM 公司的 J. Cooley 和普林斯顿大学及美国贝尔实验室的 J. Tukey 共同提出的**快速傅立叶变换算法: FFT 算法**
9. 1977 年，美国 Brigham Young 大学的 H. Ferguson 和 R. Forcade 提出的整数检测算法 (integer relation detection)
10. 1987 年，美国耶鲁大学的 L. Greengard 和 V. Rokhin 发明的快速多极算法 (fast multipole)

1947: George Dantzig(丹齐克), at the RAND Corporation(兰德公司), creates the simplex method for linear programming.

In terms of widespread application, Dantzig's algorithm is one of the most successful of all time: Linear programming dominates the world of industry, where economic survival depends on the ability to optimize within budgetary and other constraints. (Of course, the "real" problems of industry are often nonlinear; the use of linear programming is sometimes dictated by the computational budget.) **The simplex method is an elegant way of arriving at optimal answers.** Although theoretically susceptible to exponential delays, the algorithm in practice is highly efficient—which in itself says something interesting about the nature of computation.

George Dantzig

Dantzig with President Gerald Ford in 1976

Born	George Bernard Dantzig November 8, 1914 Portland, Oregon, US
Died	May 13, 2005 (aged 90) Stanford, California, US
Citizenship	American
Alma mater	University of Maryland (BS) University of Michigan (MS) University of California, Berkeley (PhD)

假设有n个变量和m个约束。线性规划的标准形式如下：

$$\max \sum_{1\le k\le n} c_k x_k$$

$$s.t. \quad \sum_{1\le k\le n} A_{1,k} x_k \le b_1,$$

$$\sum_{1\le k\le n} A_{2,k} x_k \le b_2,$$

$$\cdots$$

$$\sum_{1\le k\le n} A_{m,k} x_k \le b_m$$

$$x_1, x_2, \ldots, x_n \ge 0$$

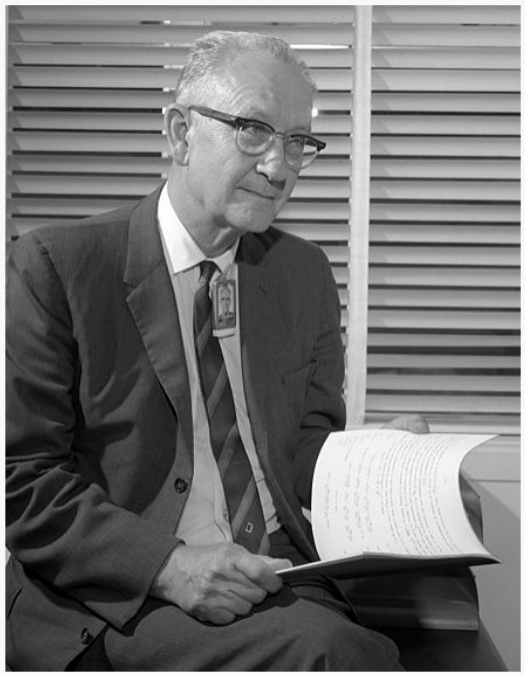
1951: Alston Householder of Oak Ridge National Laboratory formalizes the decompositional approach to matrix computations.

The ability to factor matrices into triangular, diagonal, orthogonal, and other special forms has turned out to be extremely useful.

The decompositional approach has enabled software developers to produce flexible and efficient matrix packages.
It also facilitates the analysis of rounding errors, one of the big bugbears of numerical linear algebra.

(In 1961, James Wilkinson of the National Physical Laboratory in London published a seminal paper in the Journal of the ACM, titled “Error Analysis of Direct Methods of Matrix Inversion,” based on the LU decomposition of a matrix as a product of lower and upper triangular factors.)

Alston Scott Householder



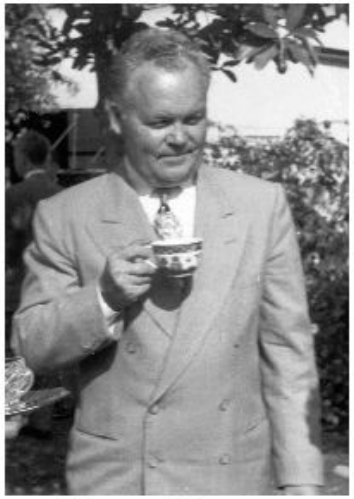
Born	5 May 1904
Died	4 July 1993 (aged 89)
Alma mater	University of Chicago
Known for	Householder transformation

1950: Magnus Hestenes, Eduard Stiefel, and Cornelius Lanczos, all from the Institute for Numerical Analysis at the National Bureau of Standards, initiate the development of Krylov subspace iteration methods.

These algorithms address the seemingly simple task of solving equations of the form **Ax = b**. The catch, of course, is that A is a huge $n \times n$ matrix, so that the algebraic answer x= b/A is not so easy to compute. (Indeed, matrix "division" is not a particularly useful concept.)

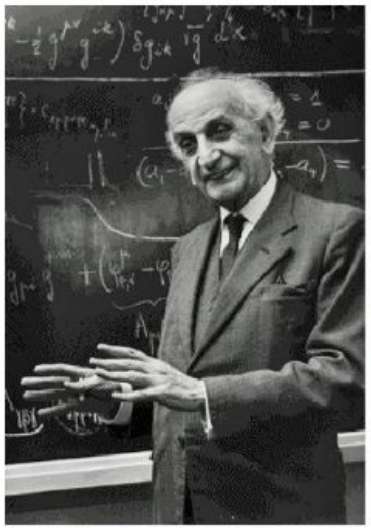
Iterative methods—such as solving equations of the form $Kx_{i+1} = Kx_i + b - Ax_i$ with a simpler matrix K that's ideally "close" to A—lead to the study of Krylov subspaces. Named for the Russian mathematician Nikolai Krylov, Krylov subspaces are spanned by powers of a matrix applied to an initial "remainder" vector $r_0 = b - Ax_0$.

Lanczos found a nifty way to generate an orthogonal basis for such a subspace when the matrix is symmetric. Hestenes and Stiefel proposed an even niftier method, known as the conjugate gradient method, for systems that are both symmetric and positive definite.



Magnus Hestenes

Eduard Stiefel (1909-1978)



Cornelius Lanczos (1893-1974)

1977: Helaman Ferguson and Rodney Forcade of Brigham Young University advance an integer relation detection algorithm (e.g. PSLQ).

The problem is an old one: **Given a bunch of real numbers, say $x_1, x_2, \ldots, x_n$, are there integers $a_1, a_2, \ldots, a_n$ (not all 0) for which $a_1x_1 + a_2x_2 + \ldots + a_nx_n = 0$?**

For n=2, the venerable Euclidean algorithm (计算最大公约数) does the job, computing terms in the continued-fraction expansion of x_1/x_2. If x_1/x_2 is rational, the expansion terminates and, with proper unraveling, gives the "smallest" integers a_1 and a_2. If the Euclidean algorithm doesn't terminate—or if you simply get tired of computing it—then the unraveling procedure at least provides lower bounds on the size of the smallest integer relation.

Ferguson and Forcade's generalization, although much more difficult to implement (and to understand), is also more powerful. Their detection algorithm, for example, has been used to find the precise coefficients of the polynomials satisfied by the third and fourth bifurcation points, $B_3 = 3.544090$ and $B_4 = 3.564407$, of the logistic map. (The latter polynomial is of degree 120; its largest coefficient is 257^30.) **It has also proved useful in simplifying calculations with Feynman diagrams in quantum field theory.**

GENERALIZATION OF THE EUCLIDEAN ALGORITHM FOR REAL NUMBERS TO ALL DIMENSIONS HIGHER THAN TWO

BY H. R. P. FERGUSON AND R. W. FORCADE

Bull. Amer. Math. Soc. (N.S.) 1(6): 912-914 (November 1979).

https://www2.lbl.gov/Science-Articles/Archive/pi-algorithm.html

PSLQ has unearthed many surprising relations in mathematics and physics, although its most startling result may well be a simple formula for calculating any binary digit of pi without calculating the digits preceding it. Before PSLQ, mathematicians had not thought that such a digit-extraction algorithm for pi was possible.

$$\pi = \sum_{k=0}^{\infty} \frac{1}{16^k}\left[\frac{4}{8k+1} - \frac{2}{8k+4} - \frac{1}{8k+5} - \frac{1}{8k+6}\right]$$

A SIMPLE FORMULA DISCOVERED WITH PSLQ MAKES IT POSSIBLE TO CALCULATE THE NTH BINARY DIGIT OF PI WITHOUT COMPUTING ANY OF THE FIRST N-1 DIGITS, AND DO THE COMPUTATION WITH VERY LITTLE COMPUTING POWER.

Using the remarkably simple formula, even a personal computer can calculate pi's millionth binary digit in about 60 seconds. Most applications of PSLQ, however, require much more computing power and must employ much greater numerical precision than the standard 16-digit, 64-bit, floating-point arithmetic available on most computers.

https://arxiv.org/abs/2103.06345

Empirical determinations of Feynman integrals using integer relation algorithms

Kevin Acres, David Broadhurst

Integer relation algorithms can convert numerical results for Feynman integrals to exact evaluations, when one has reason to suspect the existence of reductions to linear combinations of a basis, with rational or algebraic coefficients. Once a tentative reduction is obtained, confidence in its validity is greatly increased by computing more decimal digits of the terms and verifying the stability of the result. Here we give examples of how the PSLQ and LLL algorithms have yielded remarkable reductions of Feynman integrals to multiple polylogarithms and to the periods and quasi-periods of modular forms. Moreover, these algorithms have revealed quadratic relations between Feynman integrals. A recent application concerning black holes involves quadratic relations between combinations of Feynman integrals with algebraic coefficients.

1987: Leslie Greengard and Vladimir Rokhlin of Yale University invent the fast multipole algorithm.

This algorithm overcomes one of the biggest headaches of **N-body simulations**: the fact that accurate calculations of the motions of N particles interacting via gravitational or electrostatic forces (think stars in a galaxy, or atoms in a protein) would seem to require O(N^2) computations—one for each pair of particles.

The fast multipole algorithm gets by with O(N) computations. It does so by using multipole expansions (net charge or mass, dipole moment, quadrupole, and so forth) to approximate the effects of a distant group of particles on a local group. A hierarchical decomposition of space is used to define ever-larger groups as distances increase. **One of the distinct advantages of the fast multipole algorithm is that it comes equipped with rigorous error estimates, a feature that many methods lack.**

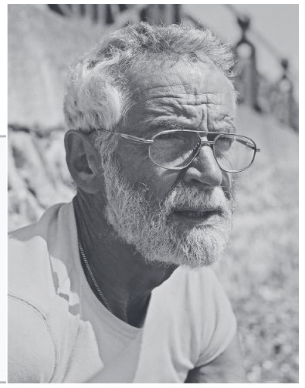
https://arxiv.org/abs/2012.02207

Fast Multipole Methods for N-body Simulations of Collisional Star Systems

Diptajyoti Mukherjee, Qirong Zhu, Hy Trac, Carl L. Rodriguez

Direct N-body simulations of star clusters are accurate but expensive, largely due to the numerous $\mathcal{O}(N^2)$ pairwise force calculations. To solve the post-million-body problem, it will be necessary to use approximate force solvers, such as tree codes. In this work, we adapt a tree-based, optimized Fast Multipole Method (FMM) to the collisional N-body problem. The use of a rotation-accelerated translation operator and an error-controlled cell opening criterion leads to a code that can be tuned to arbitrary accuracy. We demonstrate that our code, Taichi, can be as accurate as direct summation when $N > 10^4$. This opens up the possibility of performing large-N, star-by-star simulations of massive stellar clusters, and would permit large parameter space studies that would require years with the current generation of direct summation codes. Using a series of tests and idealized models, we show that Taichi can accurately model collisional effects, such as dynamical friction and the core-collapse time of idealized clusters, producing results in strong agreement with benchmarks from other collisional codes such as NBODY6++GPU or PeTar. Parallelized using OpenMP and AVX, Taichi is demonstrated to be more efficient than other CPU-based direct N-body codes for simulating large systems. With future improvements to the handling of close encounters and binary evolution, we clearly demonstrate the potential of an optimized FMM for the modeling of collisional stellar systems, opening the door to accurate simulations of massive globular clusters, super star clusters, and even galactic nuclei.

1961 QR算法：计算矩阵特征值



John Francis in July 2008

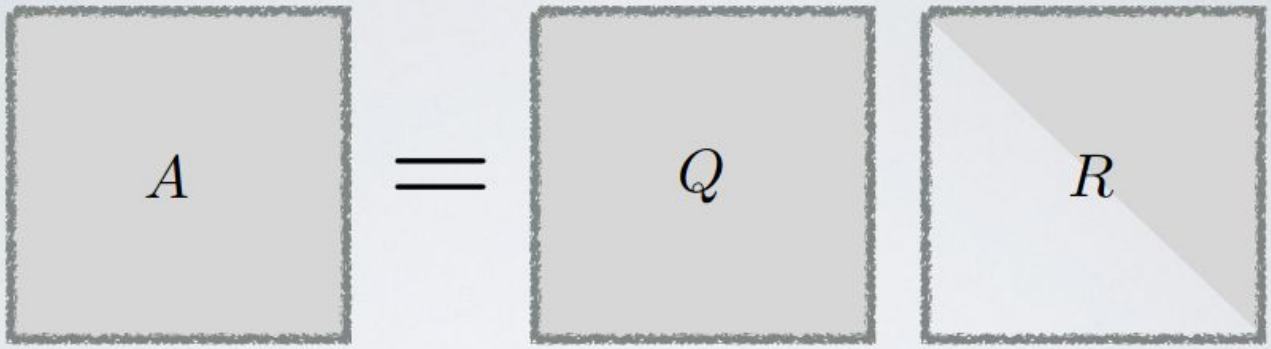
John G.F. Francis	
Born	1934 London
Known for	QR algorithm

John G.F. Francis (born 1934) is an English computer scientist, who in 1961 published the QR algorithm for computing the eigenvalues and eigenvectors of matrices,[1] which has been named as one of the ten most important algorithms of the twentieth century.[2][3] The algorithm was also proposed independently by Vera N. Kublanovskaya of the Soviet Union in the same year.[4]

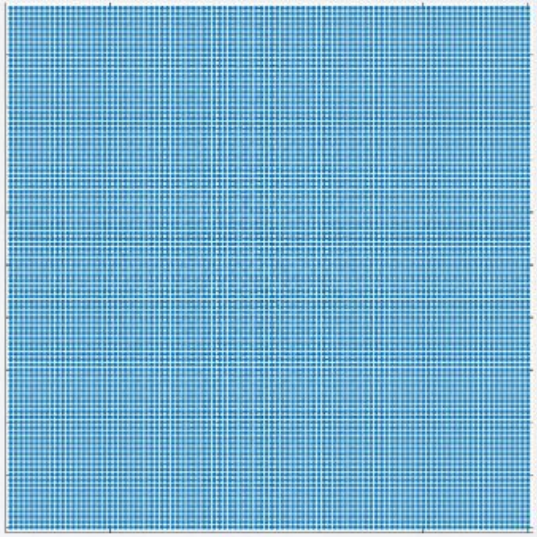
Francis was born in London in 1934. In 1954 he worked for the National Research Development Corporation (NRDC). In 1955–1956 he attended Cambridge University, but did not complete a degree. He then returned to the NRDC, where he served as assistant to Christopher Strachey. At this time he devised the QR transformation. In 1961 he left the NRDC to work at Ferranti Corporation, Ltd. and then at the University of Sussex. Subsequently, he had positions with various industrial organizations and consultancies. His interests encompassed artificial intelligence, computer languages, and systems engineering, although he never returned to the field of numerical computation.[5]

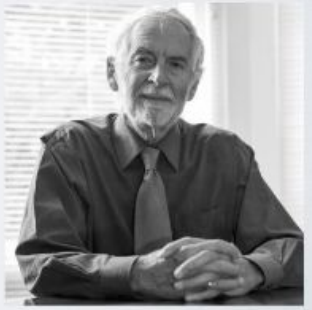
By 1962, Francis had left the field of numerical analysis, and subsequently had no idea of the impact his work on the QR algorithm had had, until re-contacted by Gene Golub and Frank Uhlig in 2007, by which time he was retired and living in Hove, England (near Brighton).[5] Still in good health, he was the opening speaker at a mini-symposium that marked 50 years of the QR algorithm, held at the 23rd Biennial Conference on Numerical Analysis in Glasgow in June 2009.[6] Francis was awarded a University of Sussex honorary doctorate in July 2015.[7]

HOW DOES IT WORK?




```
A = symmetric
for k = 1,2,...
    A = Q*R
    A = R*Q
end
```



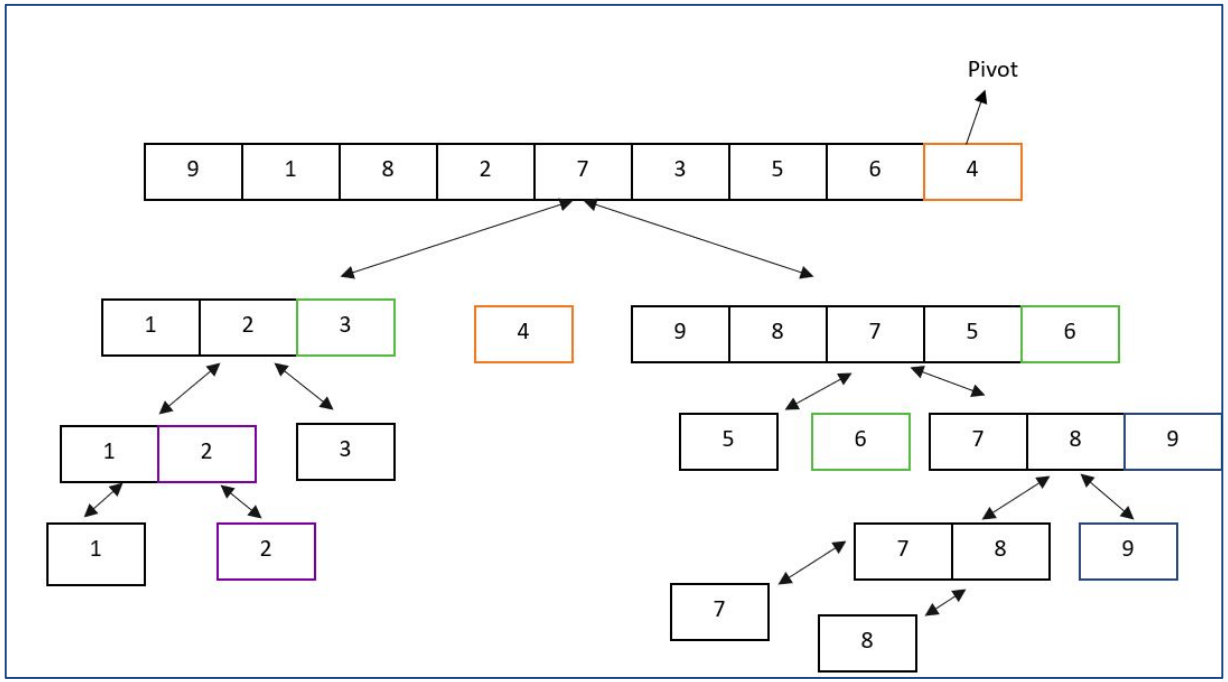


Francis

The final diagonal matrix contains all the eigenvalues

1959 Quicksort 算法

https://www.studytonight.com/python-programs/python-program-for-quicksort



Sir
Tony Hoare
FRS FREng

Tony Hoare in 2011

Born	Charles Antony Richard Hoare 11 January 1934 (age 88) Colombo, British Ceylon

on average, the algorithm takes O (n log n) comparisons to sort *n* items. In the worst case, it makes O (n^2) comparisons.

C. ANTONY ("TONY") R. HOARE

United Kingdom – 1980

1980年度图灵奖

CITATION

For his fundamental contributions to the definition and design of programming languages.

十个算法其他的名单

Top Ten Algorithms Class 1

John Burkardt
Department of Scientific Computing
Florida State University

.....

http://people.sc.fsu.edu/~jburkardt/classes/tta_2015/class01.pdf

- You left out my field of interest (data mining)
- These are very "20th Century" algorithms.
- Fortran is not an algorithm!
- This list is boring!
- The algorithms we use every day aren't here.

十个算法其他的名单: Dan Givoli (以色列, 计算力学)

1. **the Finite Element Method (including the Boundary Element Method);**
2. Iterative Linear Algebraic Solvers, include Krylov Spaces, Conjugate Gradient Methods, and GMRES;
3. Algebraic Eigenvalue Solvers, including the Lanczos and QR methods;
4. Matrix Decomposition Methods, including spectral and polar decomposition;
5. Finite Difference Methods for Wave Problems, including the methods of Newmark, Lax-Wendroff, Hilbert-Hughes-Taylor, the shock wave techniques of Godunov, upwinding and flux-splitting;
6. Nonlinear Algebraic Solvers, including Quasi Newton methods such as BFGS, and arclength or continuation methods;
7. the Fast Fourier Transform;
8. Nonlinear Programming, in particular, Quadratic Programming
9. **Soft Computing Methods, such as neural networks, genetic algorithms, and fuzzy logic.**
10. Multiscale methods, including the multigrid method and wavelets.

Dan Givoli: The Top 10 Computational Methods of the 20th Century, IACM Expressions, Number 11, September 2001, pages 5-9.

9. Soft Computing Methods

Traditionally, CM has been based on 'rigorous' classical mathematical procedures that draw on PDE theory, theoretical mechanics, numerical analysis, functional analysis, etc. However, since the early 80's new families of computational methods, which are sometimes collectively termed "soft computing" methods, have been applied. These types of schemes are based on a heuristic approach rather than on rigorous mathematics and draw on concepts of Artificial Intelligence (AI). Despite the fact that these methods were initially received with suspicion, they have turned.out in many cases to be surprisingly powerful, and their use in various areas of CM keep increasing. Three main techniques are Neural Networks, Genetic Algorithms and Fuzzy Logic. All three can be thought of as general optimisation techniques, but they are based on totally different methodologies.

Traces of soft computing ideas can be found already in the 40's. Pioneers include McCulloch and Pitts in Neural Networks, Holland in Genetic Algorithms and Zadeh in Fuzzy Logic - although some claim that Fuzzy Logic was invented by Buddha! In the 60's and 70's the area was advanced by computer scientists, but only since the early 80's application of soft computing methods in CM have started to appear.

Neural Network: 神经网络
Genetic Algorithm: 遗传算法
Fuzzy Logic: 模糊逻辑

Buddha

十个算法其他的名单：Data Mining List

1. C4.5
2. k-means clustering
3. Support vector machines
4. The Apriori algorithm
5. The EM algorithm (expectation maximization)
6. PageRank
7. AdaBoost (ensemble learning)
8. kNN: k-nearest neighbors classification
9. Naive Bayes
10. CART: Classification and Regression Trees

新方法层出不穷：CNN，GNN，Point Cloud…

十个算法其他的名单：George Dvorsky

The 10 Algorithms That Dominate Our World

By George Dvorsky | 5/22/14 1:26PM | Comments (155)

The importance of algorithms in our lives today cannot be overstated. They are used virtually everywhere, from financial institutions to dating sites. But some algorithms shape and control our world more than others — and these ten are the most significant.

1. Google Search
2. Facebook News Feed
3. OKCupid Date Matching
4. NSA Data collection, interpretation, encryption
5. "You May Also Enjoy..."
6. Google AdWords
7. High Frequency Stock Trading
8. MP3 compression
9. IBM's CRUSH (Crime Reduction Using Statistical History)
10. Auto-Tune

好的数值算法的特点

- 面向计算机，提供切实可行的算法。只能包括计算机能够直接处理的加减乘除运算、逻辑运算、以及内置的简单函数计算等。
- 能任意逼近，并有可靠的理论分析(收敛性、稳定性、误差分析)，能达到精度要求，对近似算法要保证收敛性和稳定性。
- 省时间、省资源，并有良好的计算复杂性。计算复杂性是指算法所包含的运算次数和所需的储存量。好的算法计算效率高、计算复杂度低(耗时少，存储小)。
- 多次广泛的上机试验证明算法稳定、高效。

简单来说，好的数值算法本质上有三个要求：**好，快，省**。好，指算的准确，误差小，计算效果好；快，指计算步骤少，效率高；省，指计算的时间和存储代价小。【参考书】N.J. Higham. *Accuracy and Stability of Numerical Algorithms*. SIAM, Philadelphia, PA, 1996.

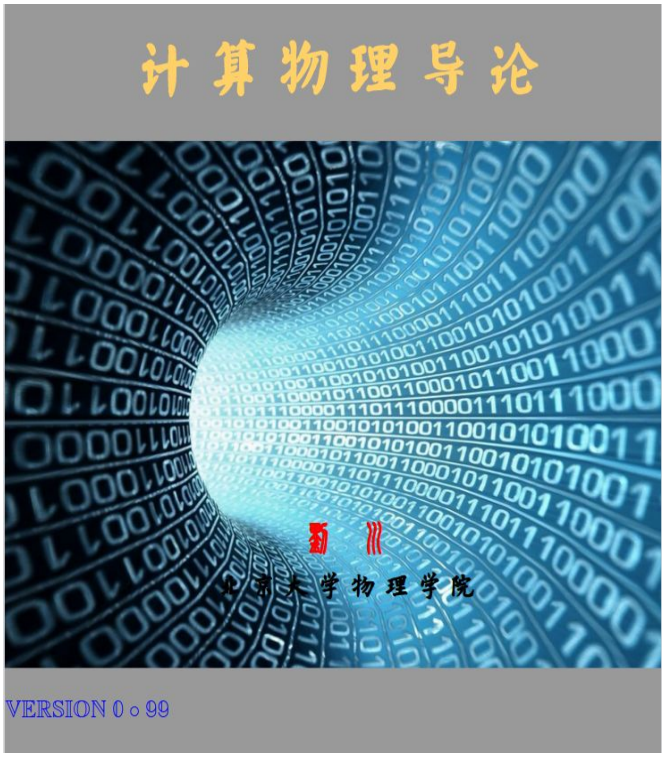
- 国内外各个大学的计算物理(或者以其他名称出现但实际上与计算物理等价)课程是所有课程中**差异性最大的一门课程**。我们这个课程经过讨论后形成的共识是，计算物理课程**主要侧重于物理学各个领域都会遇到的、具有普遍性的数值问题**。
- 而一些更加具体的、仅仅涉及到某个物理学领域的问题则可以放在更加专门的计算物理+ 的课程中。

- 计算物理当然是需要利用计算机进行求解的问题。这就涉及到人与机器的结合等多个问题：用什么机器，用什么语言或者用什么软件等等。**在计算物理中，我们更侧重于问题的基本解决的思路**(也就是算法方面更侧重一些)，至于说该问题的求解用什么语言则交给同学们自己选择。

- 我们课程的主要目并不是教会同学们如何使用某个具体软件包，而是希望让大家了解数值计算的一些基本规则和方法。诚然，多数目前的商业软件包都提供了不错的用户界面，但是本课程的目的是让大家了解一下这些界面后面的一些东西。**在你以后面对完全不同的应用时，可以知道如何去求解一个全新的数值问题。**

1. “计算 ”介绍
2. 数值计算基础
3. 线性方程组求解
4. 内插与函数的计算
5. 数值积分
6. 方程求根与函数极值
7. 本征值与本征矢量

上半部分

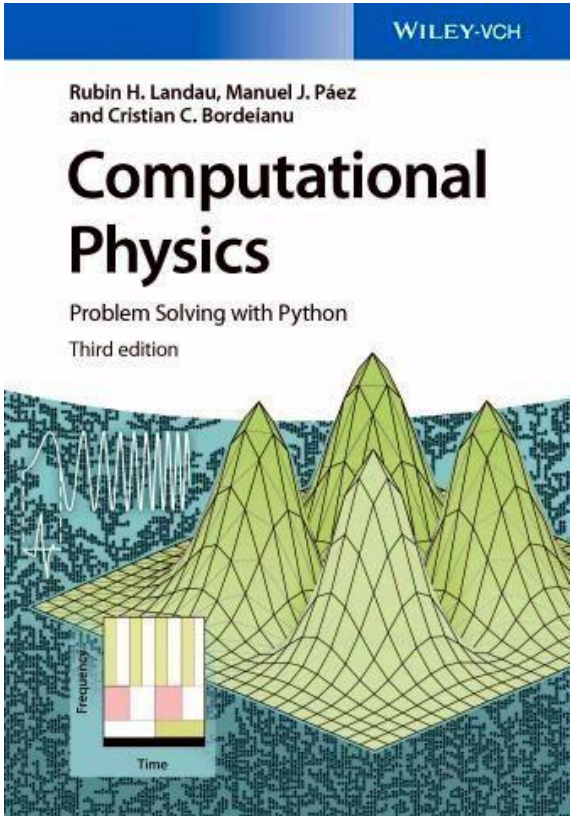


参考材料:

W.H. Press, S.A. Teukolsky, W.T. Vetterling and B.P. Flannery: **Numerical Recipes: The art of scientific computing**, 3rd Ed., Cambridge University Press, 2007.
R. L. Burden and J. D. Faires, **Numerical Analysis**, 9th ed., Brooks/Cole, Cengage Learning, 2011.
L. R. Scott, **Numerical Analysis**, Princeton University Press, 2011.

1. **常微分方程**
2. **偏微分方程**
3. **快速傅里叶变换**
4. **随机数**
5. **蒙特卡洛方法**
6. **有限元方法**
7. 机器学习初步

下半部分



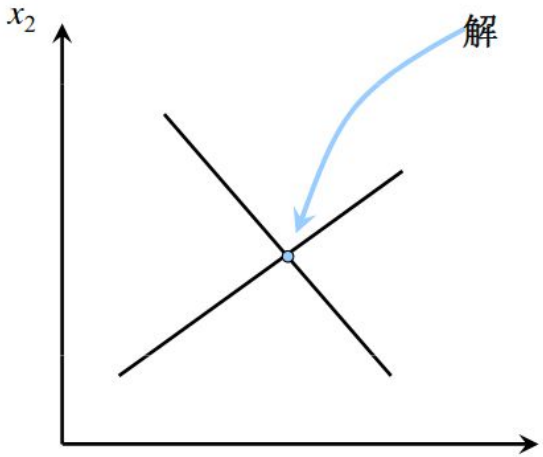
Landau Book

参考材料：

科学出版社，计算物理学，刘金远等
世界图书出版公司， An Introduction to Computational Physics， Tao Pang
科学出版社，计算物理学，马文淦
世界图书出版公司， A First Course in Computational Physics and Object-Oriented Programming with C++，David Yevick

线性代数方程组（System of Linear Algebraic Equations）

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 &= c_1 \\ a_{21}x_1 + a_{22}x_2 &= c_2 \end{aligned}$$

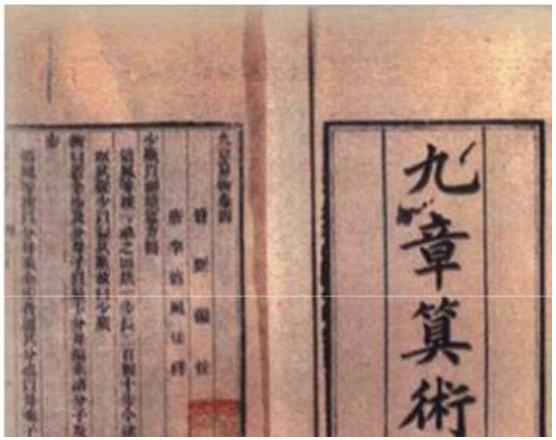


A.X=b
A可以是巨大矩阵

问：今有
上禾三秉，中禾二秉，下禾一秉，实三十九斗；
上禾二秉，中禾三秉，下禾一秉，实三十四斗；
上禾一秉，中禾二秉，下禾三秉，实二十六斗。
问上、中、下禾实一秉各几何？

——《九章算术》

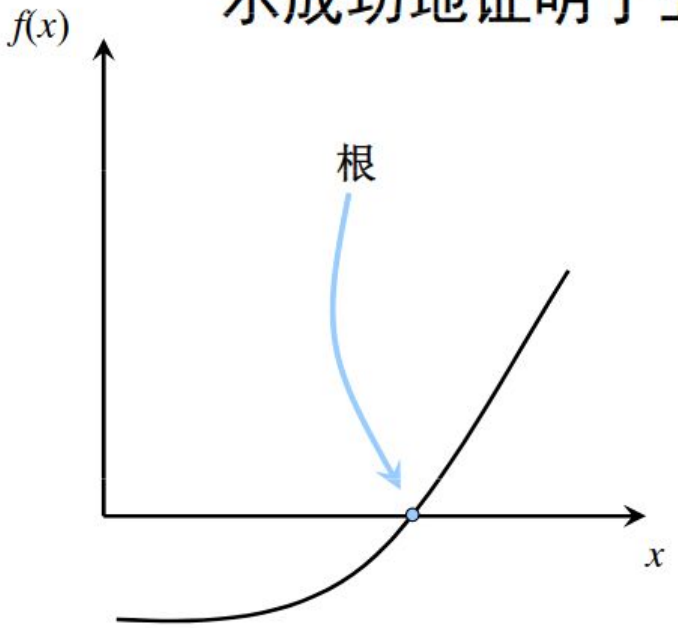
$$\begin{aligned} 3x + 2y + z &= 39 \\ 2x + 3y + z &= 34 \\ x + 2y + 3z &= 26 \end{aligned}$$



例：代数求根问题

$$f(x)=ax^2+bx+c=0 \quad \Rightarrow \quad x=\frac{-b\pm\sqrt{b^2-4ac}}{2a}$$

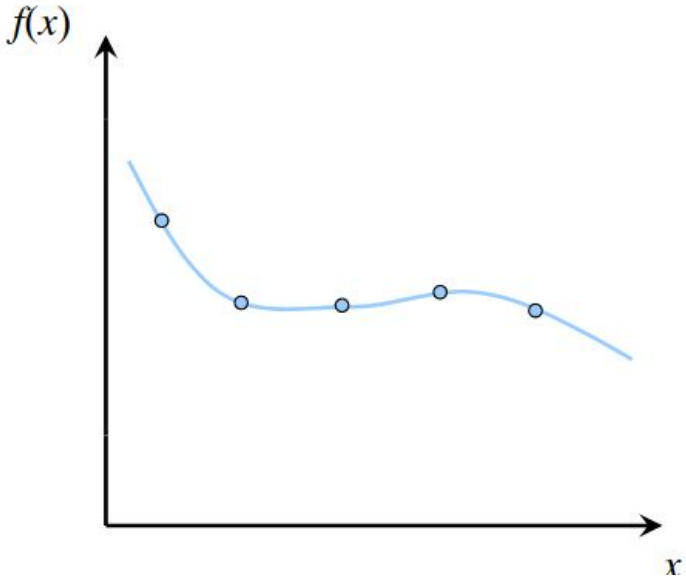
- 公元1541年意大利数学家塔尔塔利亚给出了三次方程的一般解法；公元1545年意大利数学家卡尔达诺的名著《大术》记载了费拉里的四次方程的一般解法。
- 公元1778年，法国数学大师拉格朗日提出了五次方程解不存在的猜想。公元1824年，挪威年轻数学家阿贝尔成功地证明了五次以上一般方程没有根式解。

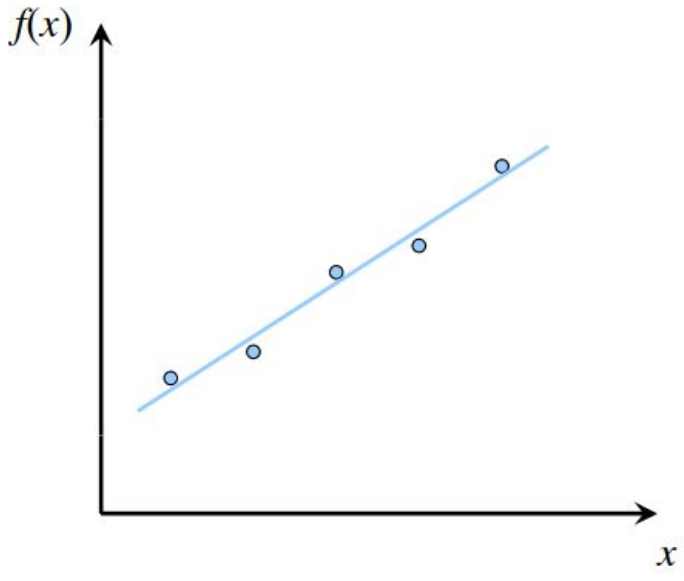


$$ax^5+bx^4+cx^3+dx^2+ex+f=0 \quad \Rightarrow x=?$$

$$\sin x+x=0 \quad \Rightarrow x=?$$

插值（Interpolation）和曲线拟合（Curve Fitting）

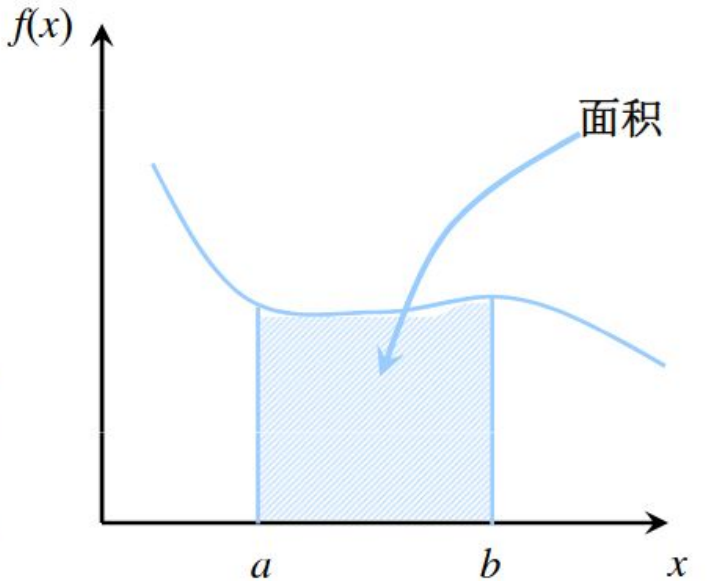




数值积分(numerical integration)和数值微分(numerical differentiation)

$$I = \int_a^b f(x)dx = F(x)\Big|_a^b$$

$$\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$

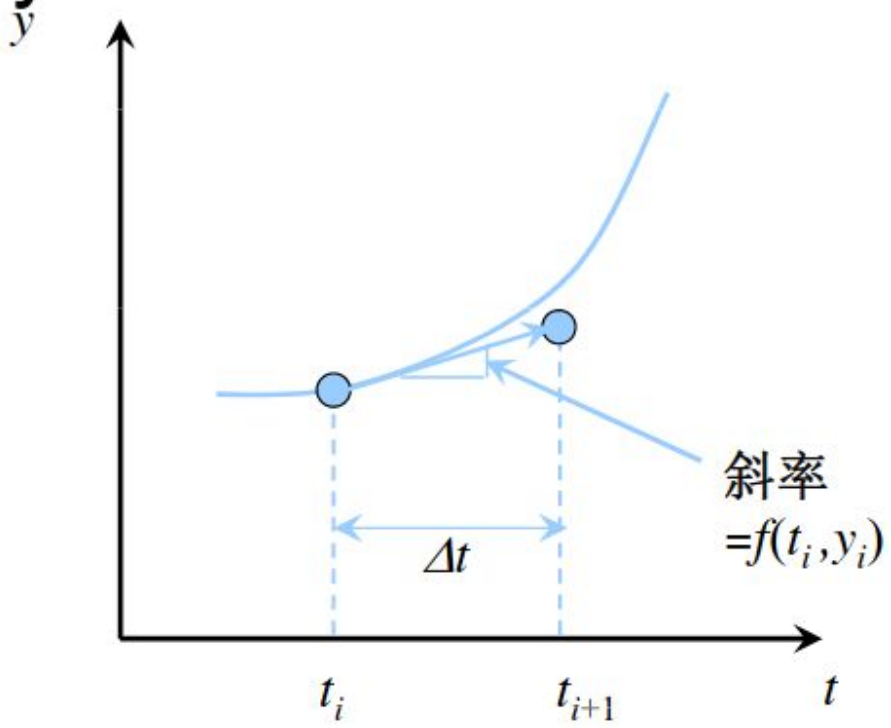


- 常微分方程（Ordinary Differential Equation）

$$\frac{dy}{dt} = f(t, y)$$

求关于自变量t的函数y

$$y_{i+1} = y_i + f(t_i, y_i)\Delta t$$



初值问题（给出积分曲线在初始点的状态）
边值问题（给出积分曲线首尾两端的状态）

1. “计算 ”介绍，常微分方程

Linux操作系统

Ubuntu

Fortran、C++简介

Euler法 示例

Python、Numpy简介

CERN ROOT数据处理软件

Histogram, bin, error-bar

Pi计算示例

作图：gnuplot、ROOT、Python

动态图示例

并行计算、版本维护

Linux之前

1983 图灵奖:
Ken Thompson，Dennis M. Ritchie
for their development of generic operating systems theory and specifically for the implementation of the UNIX operating system.

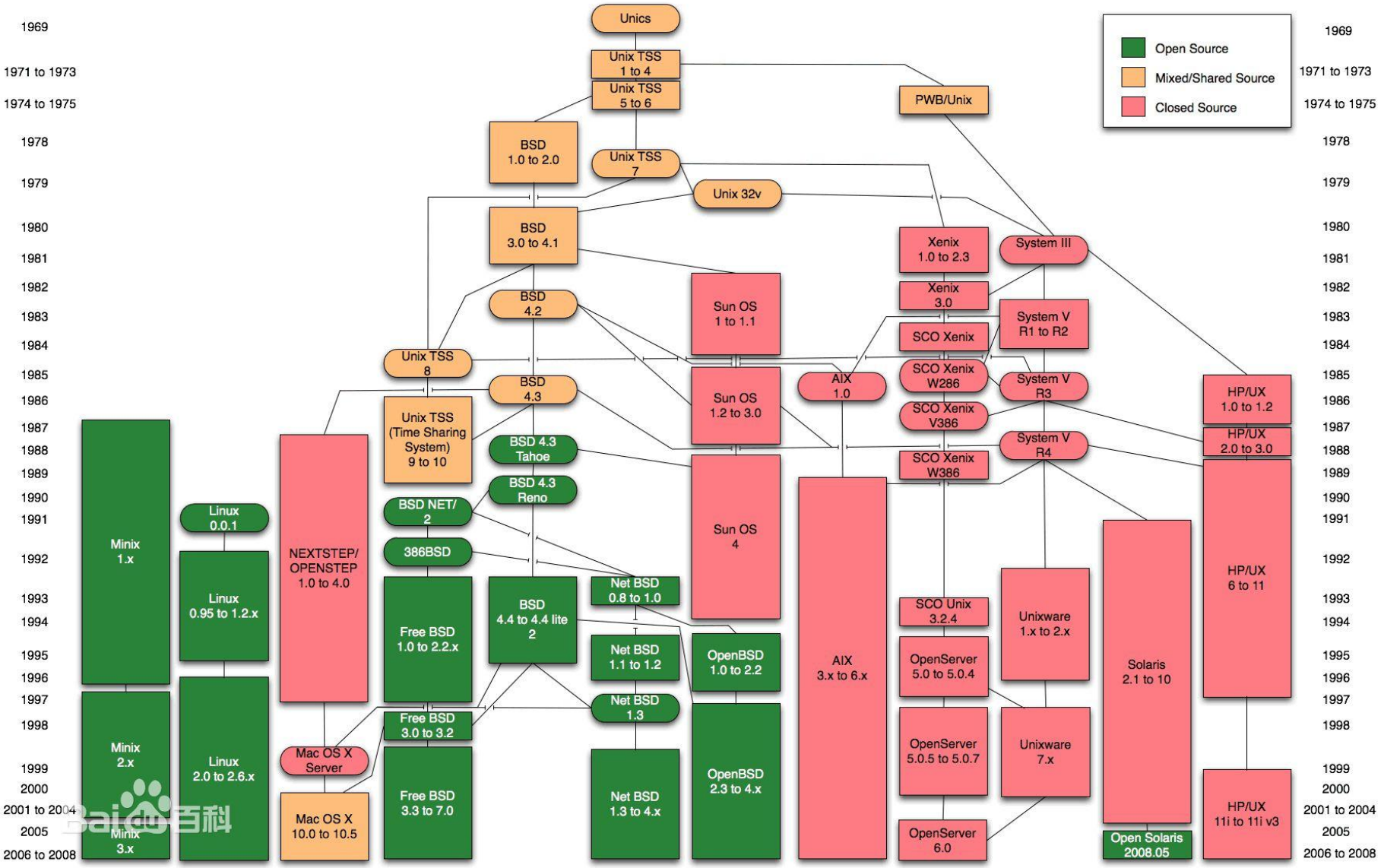
- In 80's, Microsoft's DOS (disk operating system) was the dominated OS for PC
- Apple MAC was better, but expensive
- UNIX was much better, but much, much more expensive. Only for minicomputer for commercial applications
- **People was looking for a UNIX based system, which is cheaper and can run on PC**
- Both DOS, MAC and UNIX were proprietary, i.e., the source code of their kernel is protected
- No modification is possible without paying high license fees

GNU Linux

GNU是“GNU is Not Unix”的递归缩写。

- Established in 1984 by Richard Stallman, who believes that software should be free from restrictions against copying or modification in order to make better and efficient computer programs
- GNU通用公共许可证(GNU General Public License，GPL)。即“反版权”(或称Copyleft)概念。

1991年Linus Torvalds编写出了与UNIX兼容的Linux操作系统内核并在GPL条款下发布。Linux之后在网上广泛流传，许多程序员参与了开发与修改。1992年Linux与其他GNU软件结合，完全自由的操作系统正式诞生。该操作系统往往被称为“GNU/Linux”或简称Linux。


1969
1971 to 1973
1974 to 1975
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1996
1997
1998
1999
2000
2001 to 2004
2005
2006 to 2008
Open Source
Mixed/Shared Source
Closed Source
Unics
Unix TSS 1 to 4
Unix TSS 5 to 6
PWB/Unix
BSD 1.0 to 2.0
Unix TSS 7
Unix 32v
BSD 3.0 to 4.1
Xenix 1.0 to 2.3
System III
BSD 4.2
Sun OS 1 to 1.1
Xenix 3.0
System V R1 to R2
SCO Xenix
Unix TSS 8
BSD 4.3
Sun OS 1.2 to 3.0
AIX 1.0
SCO Xenix W286
System V R3
HP/UX 1.0 to 1.2
SCO Xenix V386
HP/UX 2.0 to 3.0
Unix TSS (Time Sharing System) 9 to 10
BSD 4.3 Tahoe
System V R4
SCO Xenix W386
BSD 4.3 Reno
Minix 1.x
Linux 0.0.1
BSD NET/ 2
NEXTSTEP/ OPENSTEP 1.0 to 4.0
Sun OS 4
386BSD
Net BSD 0.8 to 1.0
Linux 0.95 to 1.2.x
Free BSD 1.0 to 2.2.x
BSD 4.4 to 4.4 lite 2
AIX 3.x to 6.x
SCO Unix 3.2.4
Unixware 1.x to 2.x
Solaris 2.1 to 10
HP/UX 6 to 11
Net BSD 1.1 to 1.2
OpenBSD 1.0 to 2.2
OpenServer 5.0 to 5.0.4
Net BSD 1.3
Free BSD 3.0 to 3.2
OpenServer 5.0.5 to 5.0.7
Unixware 7.x
Minix 2.x
Linux 2.0 to 2.6.x
Mac OS X Server
OpenBSD 2.3 to 4.x
Free BSD 3.3 to 7.0
Net BSD 1.3 to 4.x
Mac OS X 10.0 to 10.5
OpenServer 6.0
Open Solaris 2008.05
HP/UX 11i to 11i v3
Minix 3.x

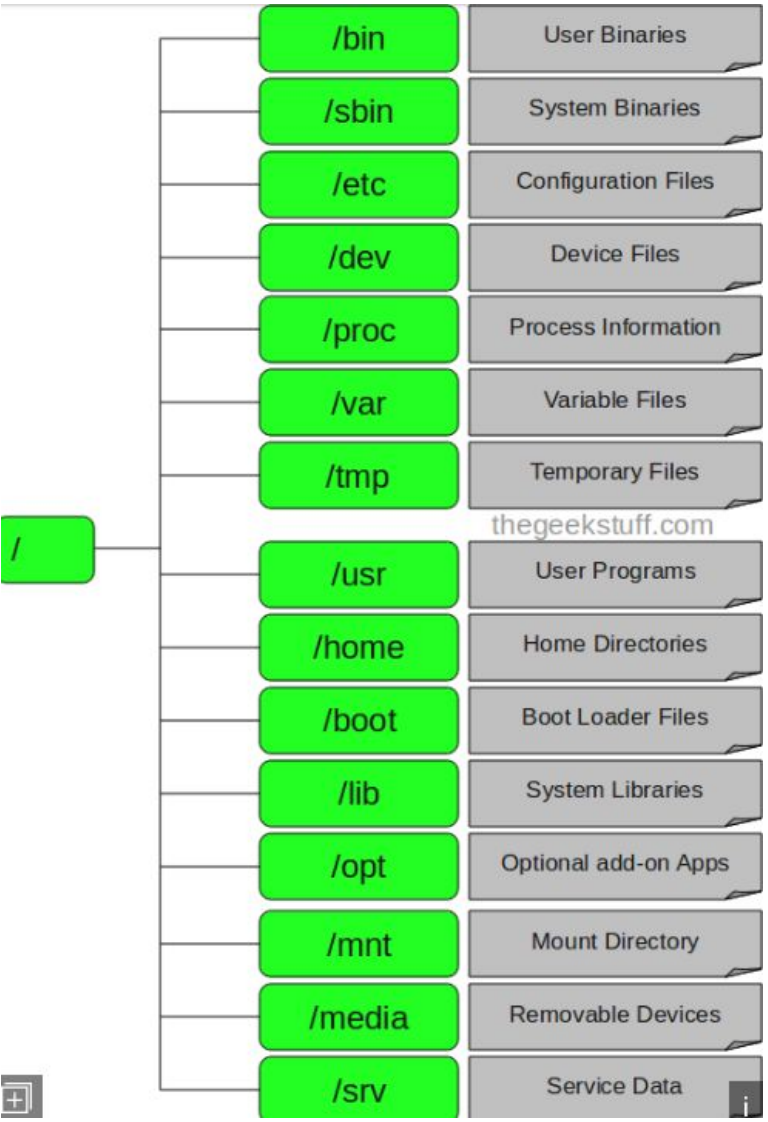
Linux系统

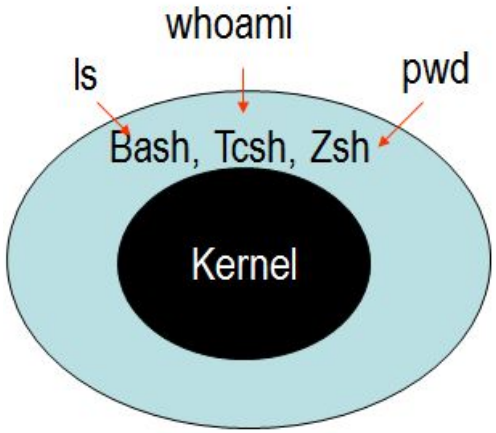
Arch Linux, CentOS, Debian, Fedora, Gentoo Linux, Linux Mint, Mageia, openSUSE and Ubuntu, together with commercial distributions such as Red Hat Enterprise Linux and SUSE Linux Enterprise Server.

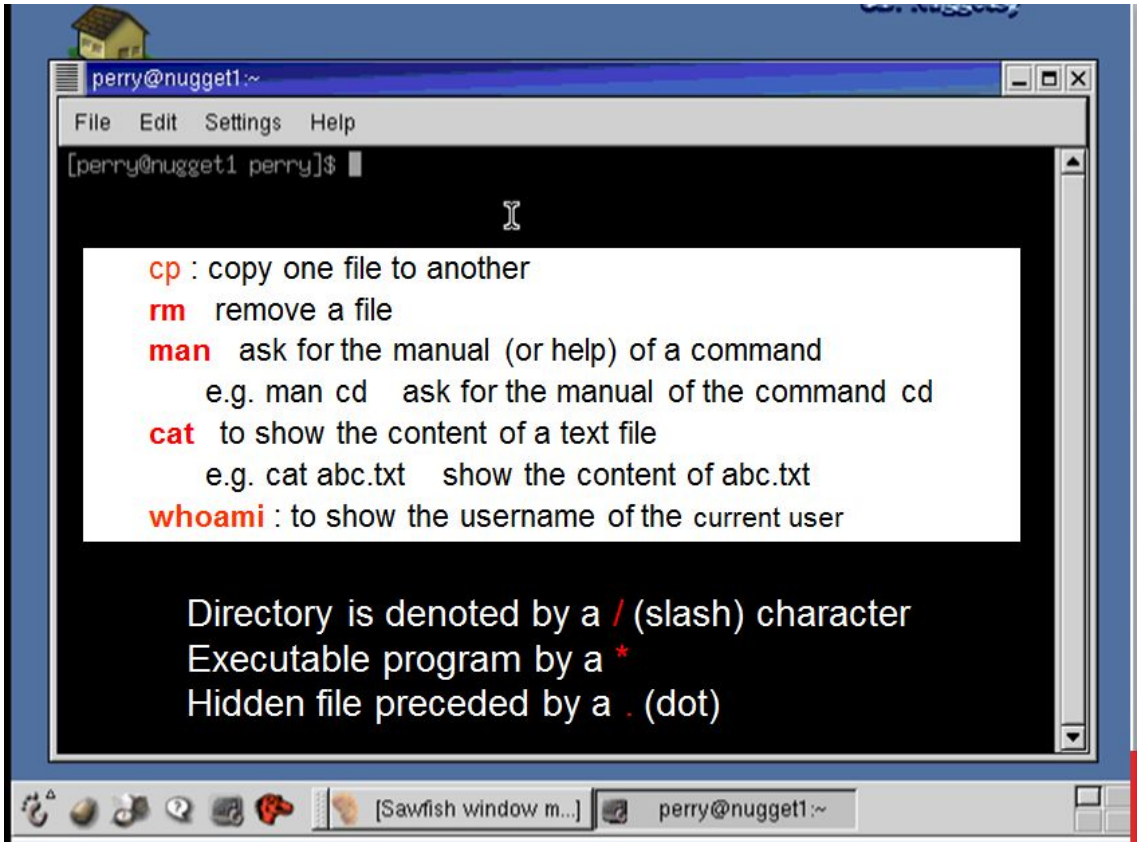
Statistics about the Linux distributions

Name	Machine
Ubuntu	39,276
Debian GNU/Linux	26,936
Fedora	10,079
Slackware Linux	9,764
SuSE Linux	9,393
Gentoo Linux	7,413
Arch Linux	4,744
CentOS	4,740
Red Hat Linux	4,672
Kubuntu	2,713
Mandrake	2,645
Mandriva	2,385
Linux Mint	2,248
unknown	2,175
openSUSE	1,750

Linux Shell以及文件系统







Ubuntu

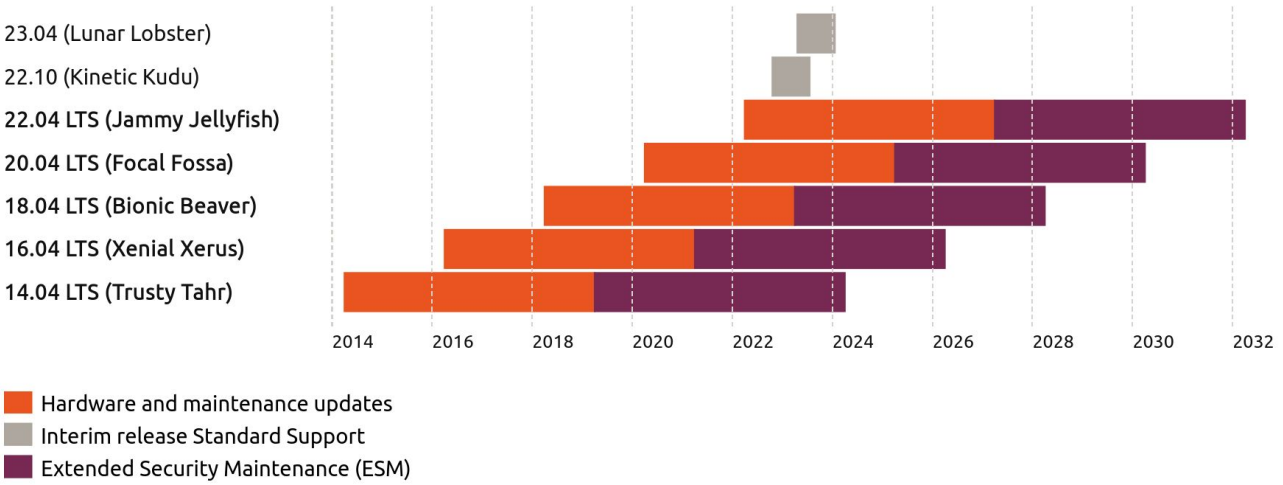
Ubuntu是一个以桌面应用为主的开源GNU/Linux操作系统，Ubuntu 是基于Debian GNU/Linux，支持x86、amd64（即x64）和ppc架构，由全球化的专业开发团队（Canonical Ltd）打造的

Arguably *the* most user-friendly version of Linux. *Huge* repository of (free) software available - by far the most of any Linux distro

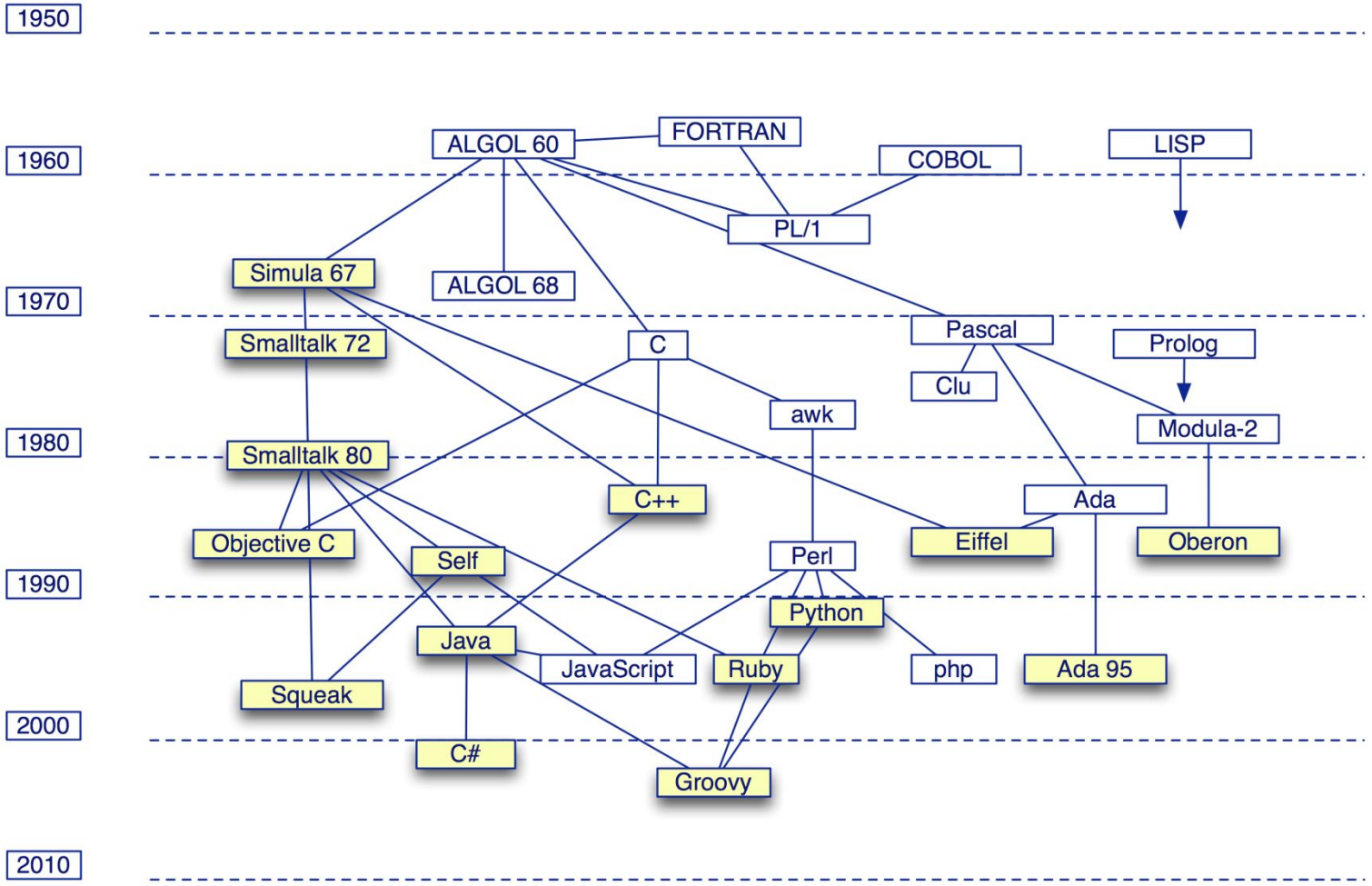
可与Windows双系统安装;可硬盘，U盘，光盘安装; 安装过程很自动

安装编译环境

sudo apt-get install build-essential
gcc, g++,….
sudo apt-get install gfortran



Object-oriented language genealogy



1979年，Bjarne Stroustrup到了Bell实验室，开始从事将C改良为带类的C（*C with classes*）的工作。1983年该语言被正式命名为C++。

Simula is considered the first object-oriented programming language. As its name suggests, Simula was designed for doing simulations, and the needs of that domain provided the framework for many of the features of object-oriented languages today.

Simula

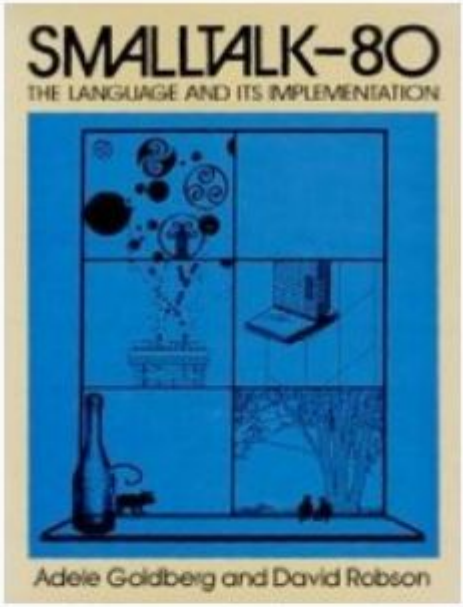
Paradigm	Object-oriented
Designed by	Ole-Johan Dahl, Kristen Nygaard
First appeared	1965
Influenced by	
	ALGOL 60
Influenced	
	Object-oriented programming languages

ALAN KAY DL

United States – 2003

CITATION

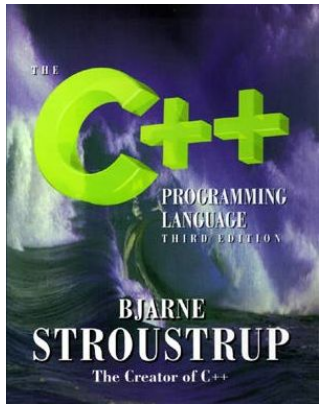
For pioneering many of the ideas at the root of contemporary object-oriented programming languages, leading the team that developed Smalltalk, and for fundamental contributions to personal computing.



Paradigm	Object-oriented
Designed by	Alan Kay, Dan Ingalls, Adele Goldberg
Developer	Alan Kay, Dan Ingalls, Adele Goldberg, Ted Kaehler, Diana Merry, Scott Wallace, Peter Deutsch and Xerox PARC
First appeared	1972; 46 years ago (development began in 1969)
Stable release	Smalltalk-80 version 2 / 1980; 38 years ago

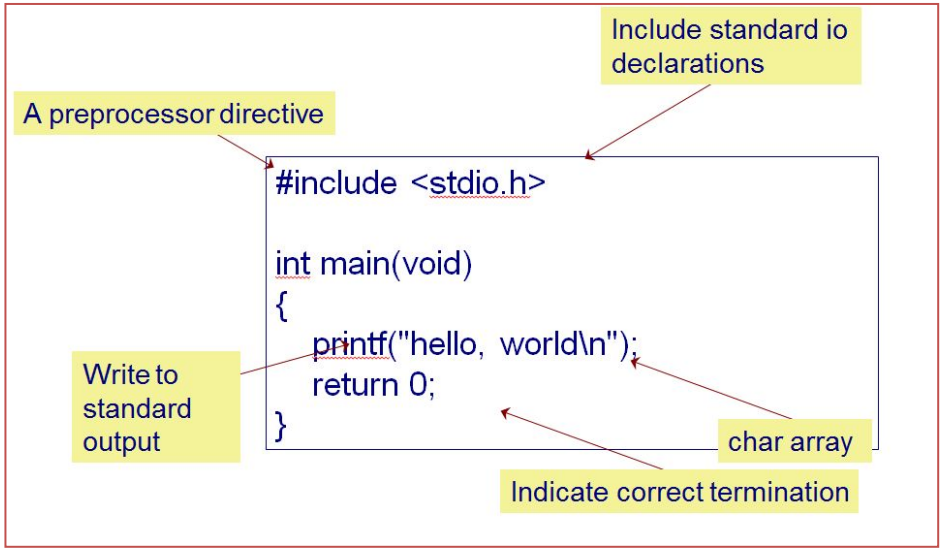
C++简介

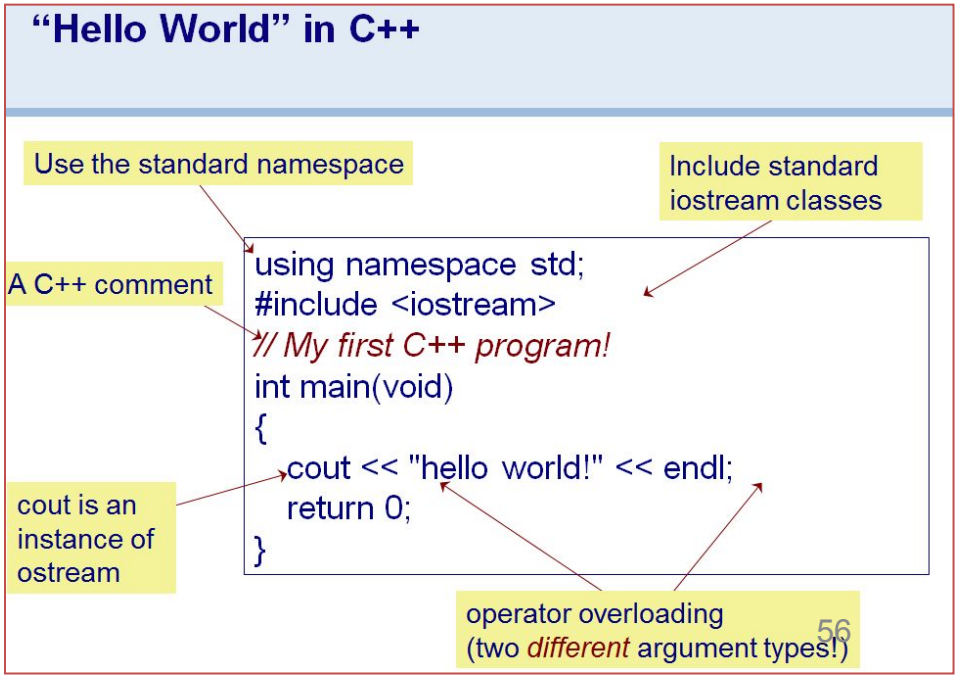
A *"better C"* that supports:
- Systems programming
- Object-oriented programming (*classes* & *inheritance*)
- Programming-in-the-large (*namespaces*, *exceptions*)
- Generic programming (*templates*)
- Reuse (large class & template libraries)



Most C programs are also C++ programs.

gcc hello.c –o hello





```
#include<iostream>
#include<algorithm>
using namespace std;
const int maxn=1e5+5;
int partition(int a[],int p,int r)
{
	int x=a[r];
	int i=p-1;
	for(int j=p;j<r;j++){
	    if(a[j]<=x)
	        swap(a[++i],a[j]);
	swap(a[i+1],a[r]);
	return i+1;
}

void quickSort(int a[],int p,int r)
{
	if(p<r)
	{ int q=partition(a,p,r);
	quickSort(a,p,q-1);
	quickSort(a,q+1,r);
	}
}
```

```
int main()
{
	int n;
	cin>>n;
	int a[maxn];
	for(int i=0;i<n;i++)
	cin>>a[i];
	quickSort(a,0,n-1);
	for(int i=0;i<n;i++)
	{
	if(i)
		cout<<" ";
	cout<<a[i];
	}
	cout<<endl;
	return 0;
}
```

```
qliphy@qliphy:~/Desktop/Teaching23/2023CP/NEW/quciksort$ g++ -w -o sort 1.c
qliphy@qliphy:~/Desktop/Teaching23/2023CP/NEW/quciksort$ ./sort
5
12
21
14
32
33
p=0
r=4
i+1=4
12 x 21 x 14 x 32 x 33
p=0
r=3
i+1=3
12 x 21 x 14 x 32 x 33
p=0
r=2
i+1=1
12 x 14 x 21 x 32 x 33
12 14 21 32 33
```

Fortran

JOHN BACKUS 1977图灵奖

United States – 1977

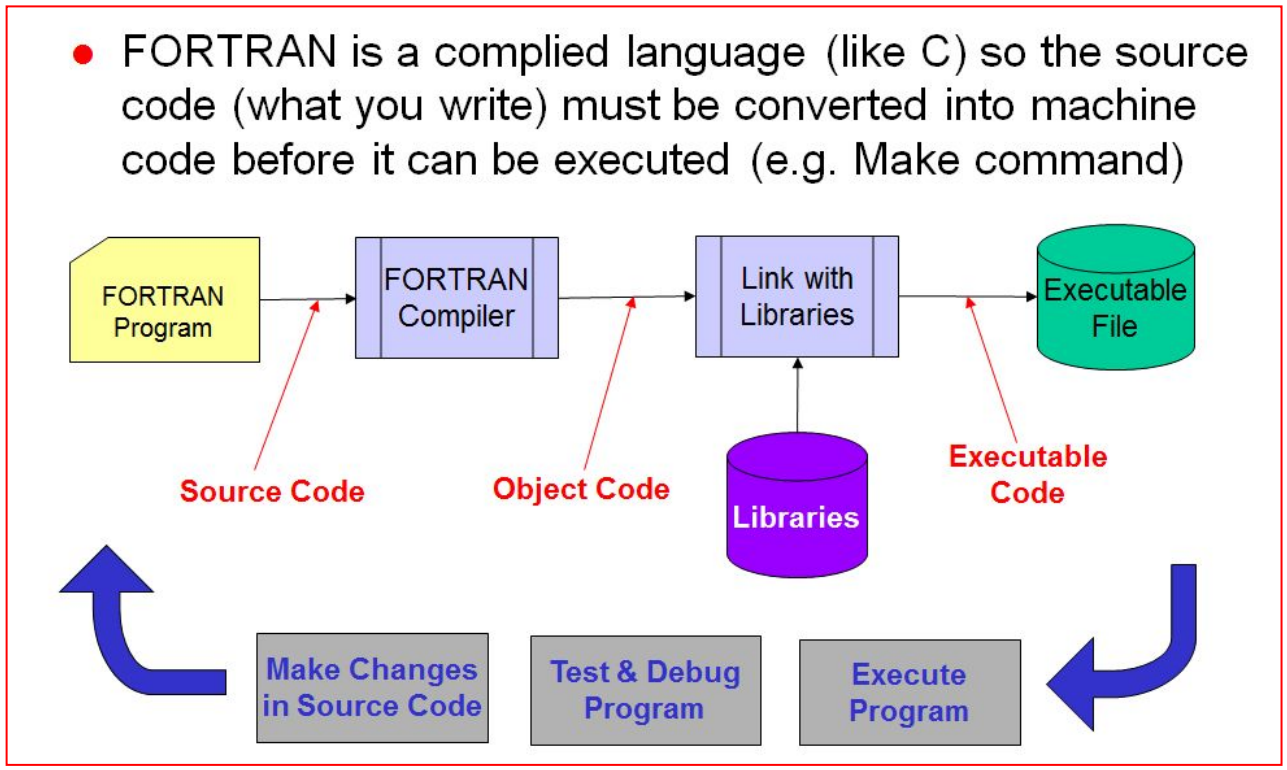
CITATION

For profound, influential, and lasting contributions to the design of practical high-level programming systems, notably through his work on FORTRAN, and for seminal publication of formal procedures for the specification of programming languages.

- One of the oldest computer languages
  - created by John Backus and released in 1957
  - designed for scientific and engineering computations
- Version history
  - FORTRAN 1957
  - FORTRAN II
  - FORTRAN IV
  - FORTRAN 66 (released as ANSI standard in 1966)
  - FORTRAN 77 (ANSI standard in 1977)
  - FORTRAN 90 (ANSI standard in 1990)
  - FORTRAN 95 (ANSI standard version)
  - FORTRAN 2003 (ANSI standard version)

Fortran

- **FORTRAN was created to solve scientific and engineering problems**
- **Introduced integer and floating point variables**
- Introduced array data types for math computations
- Introduced subroutines and subfunctions
- There is a free compiler in Unix-Linux systems
  - f77, g77 - **g95, gfortran**



Fortran 结构

- Skeleton of a program…

```
      PROGRAM MAIN
      REAL KGLO,FORC,KEL
      COMMON /STIF/KGLO(100,100)/LOAD/FORC(100)/DEF/D(100)
C     ...read in data and initialize problem...
      DO 100 IELEM=1,NELEMS
C        ...assemble global stiffness matrix...
         CALL KELEM(IELEM,KEL)
         CALL ASMBK(IELEM,KEL)
100   CONTINUE
      DO 200 ILOAD=1,NLOADS
C        ...assemble load vector...
         CALL LODVEC(ILOAD,LOAD)
200   CONTINUE
      CALL CONSTR(KDOFS)
      CALL SOLVE(NDOFS)
C     ...print out results, etc. ...
      END
```

partial list of declarations

Calculate stiffness matrix, KEL, for a single element

Add KEL to global stiffness matrix, KGLO

Construct FORC from individual loads defined in LOAD array

Must constrain problem at specified DOF's (or no solution possible)

Compute solution for displacements

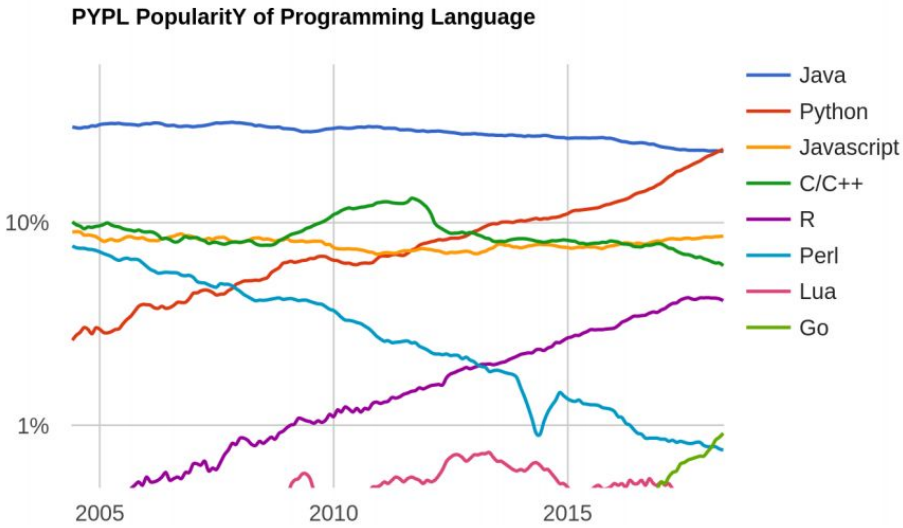
Python

- Open source general-purpose language.
- Object Oriented, Modular
- Easy to interface with C++/C/Java/Fortran
- Interactive environment
- Interpreted and therefore slower than compiled languages

Python is an interpreted high-level programming language for general-purpose programming. Created by Guido van Rossum and first released in 1991, Python has a design philosophy that emphasizes code readability, notably using significant whitespace. It provides constructs that enable clear programming on both small and large scales

斐波那契数列

```
def fib(n):
    a, b = 0, 1
    while a < n:
      print(a, end=' ')
      a, b = b, a+b
    print()
fib(1000)
```




```
$ python3.4 1.py
0 1 1 2 3 5 8 13 21 34 55 89 144 233 377 610
987
```

end=' '不换行是python3版本的用法，python2版本无法编译

http://pypl.github.io/PYPL.html

Python

```
>>> import antigravity
>>> import this
```

```
sudo apt install python3-pip
(python2: sudo apt install
python-pip)

pip3 install matplotlib
pip3 install numpy
pip3 install pandas
pip3 install scipy
pip3 install vpython

pip3 install --upgrade pip
pip3 install jupyter
jupyter notebook
```

- C++:
  - Fast
  - Compiled
  - Statically typed
    - int i = 0;
  - Access to pointers
  - Whitespace irrelevant

- python:
  - Slower
  - Interpreted
  - Dynamically typed:
    - i = 0
  - No pointers
  - Whitespace matters

Best case is to have your "human" handling with python and your hardcore computer code in C++ .
Then call the C++ code from python.
This is what scipy, numpy do, etc.

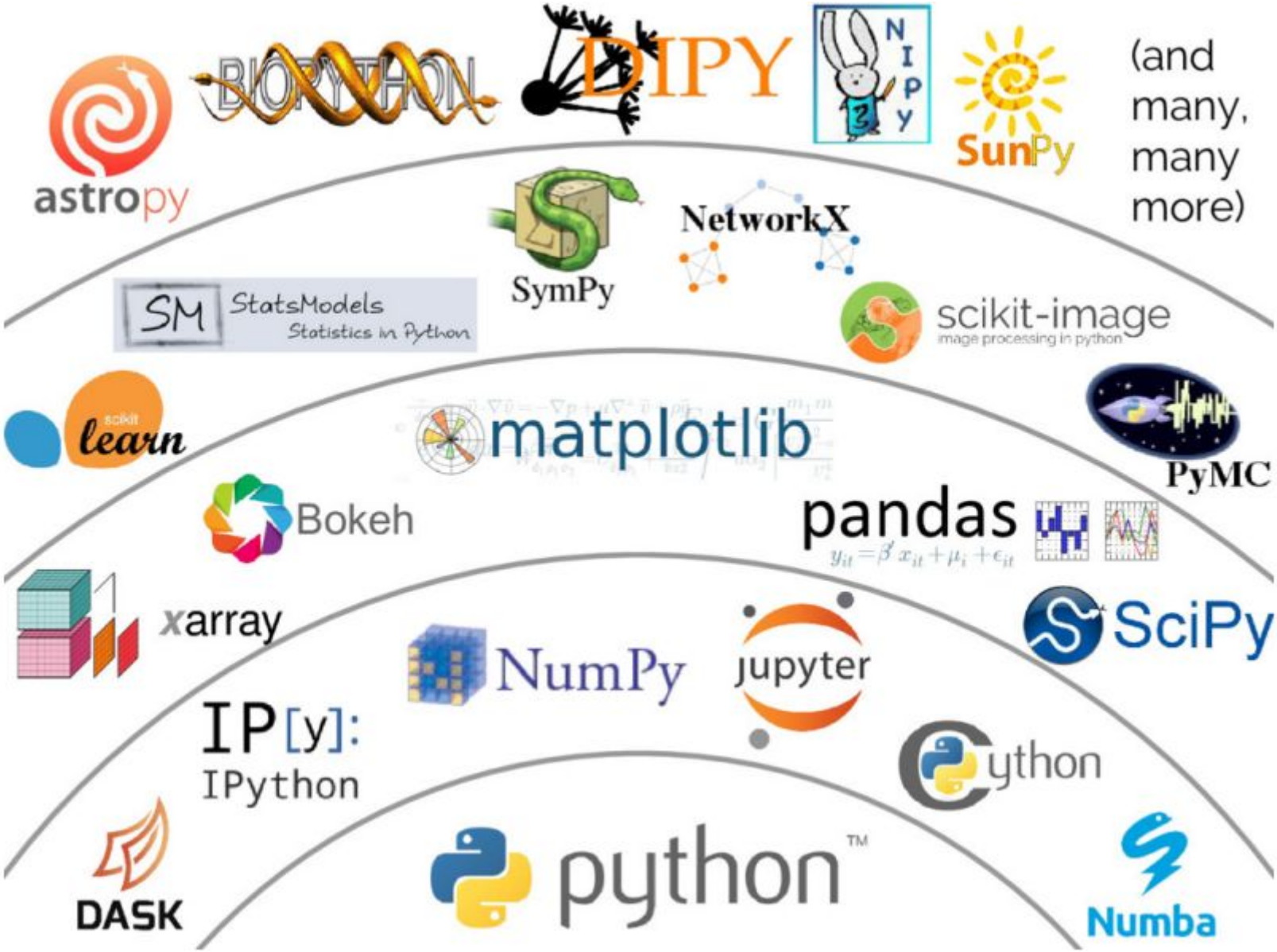
Python Example

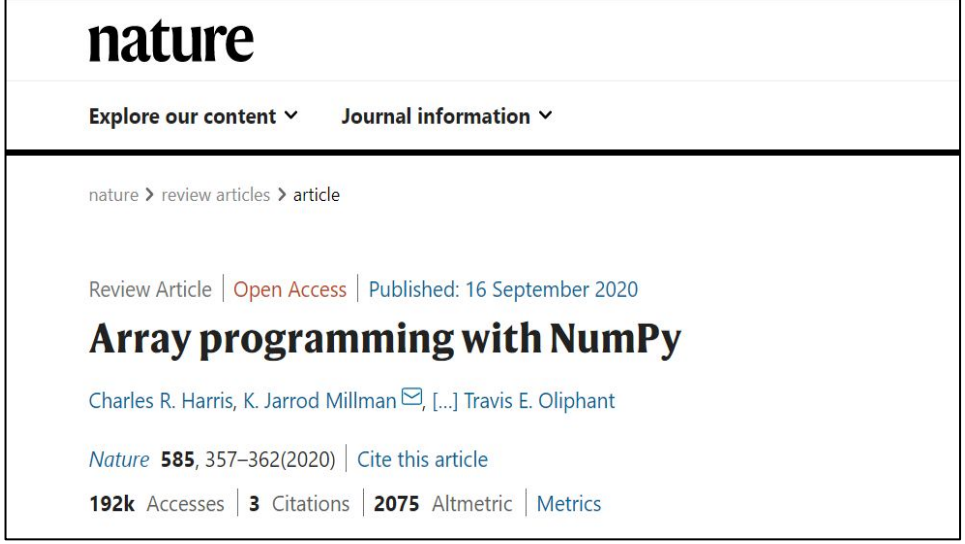
```
def partition(arr, low, high):
  # rightmost element as pivot
  pivot = arr[high]

  # pointer
  i = low - 1

  for j in range(low, high):
      if arr[j] <= pivot:
      i = i + 1
      (arr[i], arr[j]) = (arr[j], arr[i])
  (arr[i + 1], arr[high]) = (arr[high], arr[i + 1])

  # return the position
  return i + 1
```

```
# QickSort
def QuickSort(arr, low, high):
  if low < high:
      # find pivot element
      pivot = partition(arr, low, high)
      print("Intermediate:", array)
      QuickSort(arr, low, pivot - 1)
      QuickSort(arr, pivot + 1, high)

# Driver Code
array = [9, 1, 8, 2, 7, 3, 5, 6, 4]
print("The Original Array:", array)

size = len(array)
QuickSort(array, 0, size - 1)
print('The Sorted Array:', array)
```

```
qliphy@qliphy:~/Desktop/Teaching23/2023CP/NEW/quciksort$ python 1.py
('The Original Array:', [9, 1, 8, 2, 7, 3, 5, 6, 4])
('Intermediate:', [1, 2, 3, 4, 7, 8, 5, 6, 9])
('Intermediate:', [1, 2, 3, 4, 7, 8, 5, 6, 9])
('Intermediate:', [1, 2, 3, 4, 7, 8, 5, 6, 9])
('Intermediate:', [1, 2, 3, 4, 7, 8, 5, 6, 9])
('Intermediate:', [1, 2, 3, 4, 5, 6, 7, 8, 9])
('Intermediate:', [1, 2, 3, 4, 5, 6, 7, 8, 9])
('The Sorted Array:', [1, 2, 3, 4, 5, 6, 7, 8, 9])
qliphy@qliphy:~/Desktop/Teaching23/2023CP/NEW/quciksort$ vi 1.py
qliphy@qliphy:~/Desktop/Teaching23/2023CP/NEW/quciksort$ python 1.py
('The Original Array:', [12, 21, 14, 32, 33])
('Intermediate:', [12, 21, 14, 32, 33])
('Intermediate:', [12, 21, 14, 32, 33])
('Intermediate:', [12, 14, 21, 32, 33])
('The Sorted Array:', [12, 14, 21, 32, 33])
```

Python-ecosystem





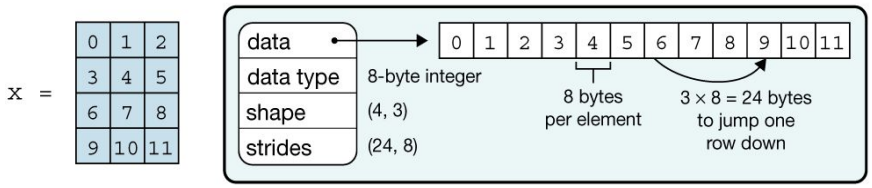
Numpy

in 2005 NumPy emerged as a 'best of both worlds' unification[7]—combining the features of Numarray with the small-array performance of Numeric and its rich C API.

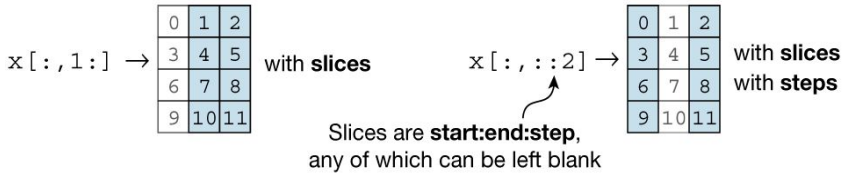
Array programming provides a powerful, compact and expressive syntax for accessing, manipulating and operating on data in vectors, matrices and higher-dimensional arrays. NumPy is the primary array programming library for the Python language. It has an essential role in research analysis pipelines in fields as diverse as physics, chemistry, astronomy, geoscience, biology, psychology, materials science, engineering, finance and economics. For example, in astronomy, NumPy was an important part of the software stack used in the discovery of gravitational waves[1] and in the first imaging of a black hole[2]. Here we review how a few fundamental array concepts lead to a simple and powerful programming paradigm for organizing, exploring and analysing scientific data. NumPy is the foundation upon which the scientific Python ecosystem is constructed. It is so pervasive that several projects, targeting audiences with specialized needs, have developed their own NumPy-like interfaces and array objects. Owing to its central position in the ecosystem, NumPy increasingly acts as an interoperability layer between such array computation libraries and, together with its application programming interface (API), provides a flexible framework to support the

Numpy

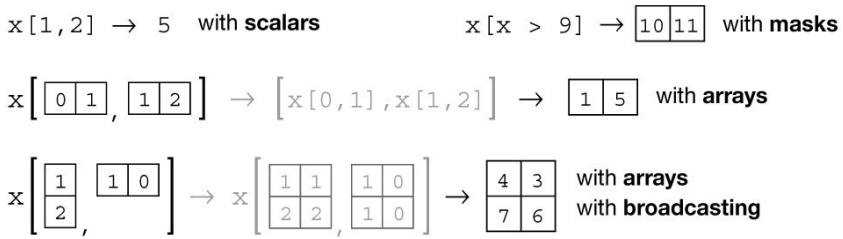
a Data structure



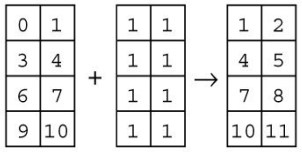
b Indexing (view)



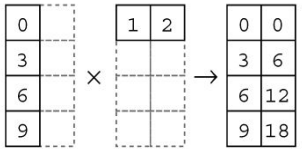
c Indexing (copy)



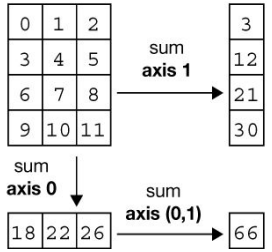
d Vectorization



e Broadcasting



f Reduction



g Example

```
In [1]: import numpy as np

In [2]: x = np.arange(12)

In [3]: x = x.reshape(4, 3)

In [4]: x
Out[4]:
array([[ 0,  1,  2],
       [ 3,  4,  5],
       [ 6,  7,  8],
       [ 9, 10, 11]])

In [5]: np.mean(x, axis=0)
Out[5]: array([4.5, 5.5, 6.5])

In [6]: x = x - np.mean(x, axis=0)

In [7]: x
Out[7]:
array([[-4.5, -4.5, -4.5],
       [-1.5, -1.5, -1.5],
       [ 1.5,  1.5,  1.5],
       [ 4.5,  4.5,  4.5]])
```

Numpy

```
import time
import numpy as np

size_of_vec = 1000
def pure_python_version():
    t1 = time.time()
    X = range(size_of_vec)
    Y = range(size_of_vec)
    Z = [X[i] + Y[i] for i in range(len(X)) ]
    return time.time() - t1
def numpy_version():
    t1 = time.time()
    X = np.arange(size_of_vec)
    Y = np.arange(size_of_vec)
    Z = X + Y
    return time.time() - t1
t1 = pure_python_version()
t2 = numpy_version()
print(t1, t2)
print("Numpy is in this example " + str(t1/t2) + " faster!")
```

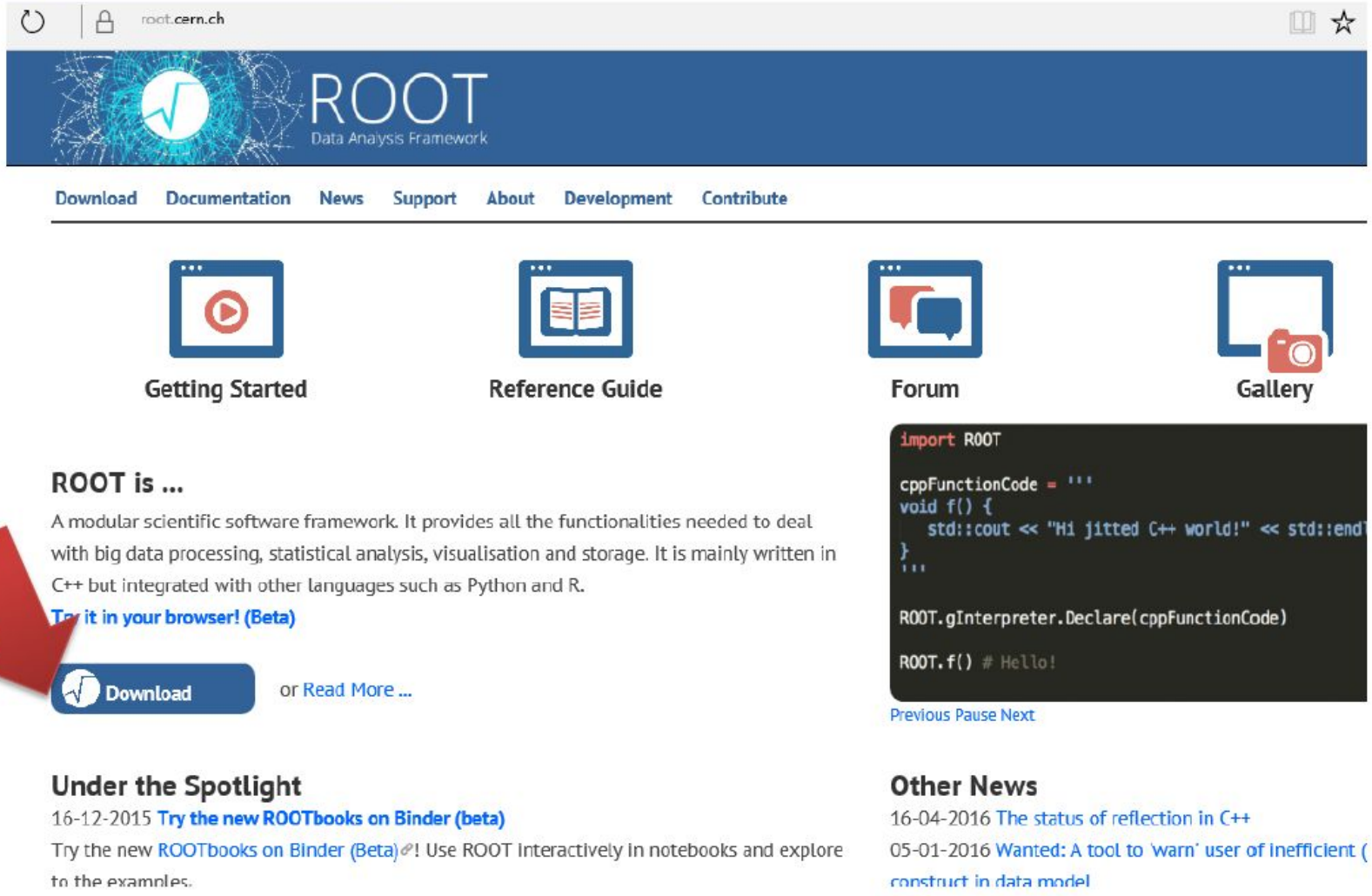
```
0.0004336833953857422 2.2649765014648438e-05
Numpy is in this example 19.147368421052633 faster!
```

CERN Root

欧洲核子中心(CERN)开发的大型科学数据处理软件

基于Cint(C/C++ interpreter, C-int)是一个C++解释器, 和GCC、VC等编译器不同,它是解释执行C++代码的

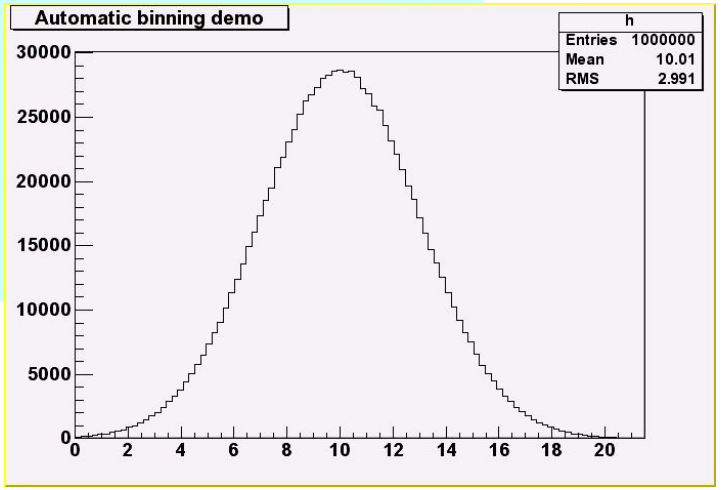
https://root.cern.ch/



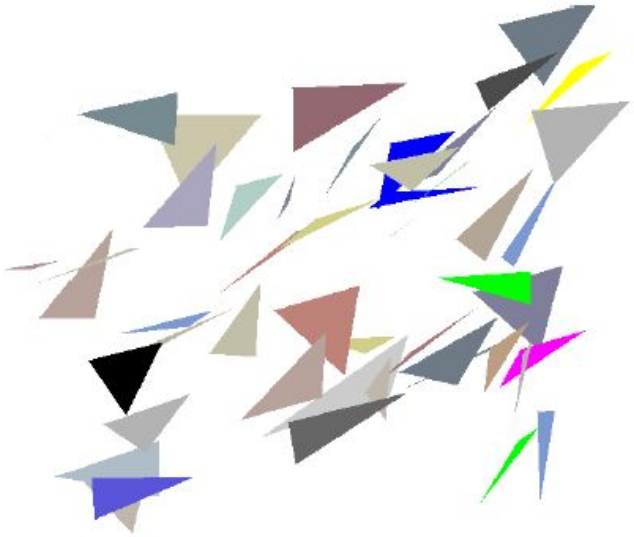
CERN Root: Histogram

Bin, Events, Mean, RMS

```
#include "TH1.h"
#include "TF1.h"

void demoauto() {
   TF1 *f1 = new TF1("f1","gaus",0,30);
   f1->SetParameters(1,10,3);
   TH1F *h = new TH1F("h","Automatic binning
demo",100,0,20);
   for (Int_t i=0;i<1000000;i++) {
      h->Fill(f1->GetRandom());
   }
   h->Draw();
}
```

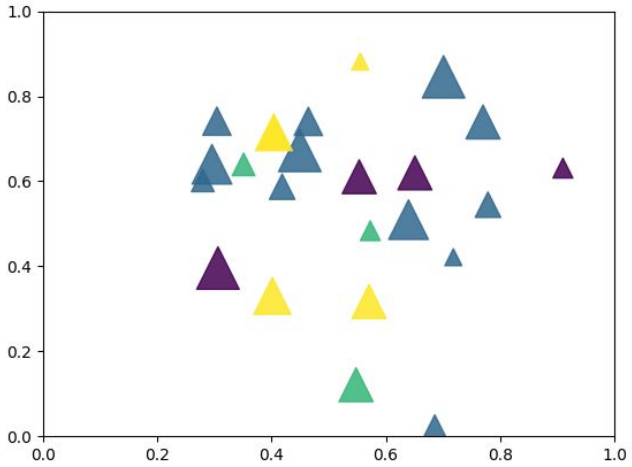


CERN Root 例1：三角图形



```
TCanvas *c1 = new TCanvas("c1","triangles",10,10,700,700);
TRandom r;
Double_t dx = 0.2; Double_t dy = 0.2;
Int_t ncolors = gStyle->GetNumberOfColors();
Double_t x[4],y[4];
TColor *c;
Int_t ci;
for (Int_t i=0;i<ntriangles;i++) {
   x[0] = r.Uniform(.05,.95); y[0] = r.Uniform(.05,.95);
   x[1] = x[0] + dx*r.Rndm(); y[1] = y[0] + dy*r.Rndm();
   x[2] = x[1] - dx*r.Rndm(); y[2] = y[1] - dy*r.Rndm();
   x[3] = x[0];               y[3] = y[0];
   TPolyLine *pl = new TPolyLine(4,x,y);
   pl->SetUniqueID(i);
   ci = ncolors*r.Rndm();
   c  = gROOT->GetColor(ci);
   c->SetAlpha(r.Rndm());
   pl->SetFillColor(ci);
   pl->Draw("f");
}
c1->AddExec("ex","TriangleClicked()");
```

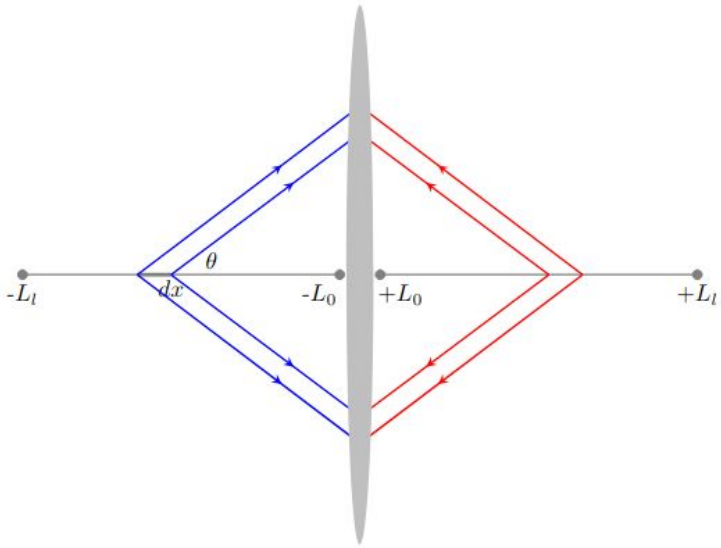
Python 画图

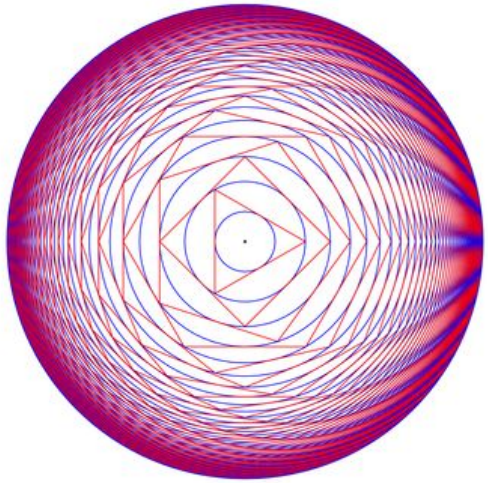



```
import math
import random
import matplotlib.pyplot as plt
# create random data
no_of_balls = 25
x = [random.triangular() for i in
range(no_of_balls)]
y = [random.gauss(0.5, 0.25) for i in
range(no_of_balls)]
colors = [random.randint(1, 4) for i in
range(no_of_balls)]
areas = [math.pi * random.randint(5, 15)**2
for i in range(no_of_balls)]
# draw the plot
plt.figure()
plt.scatter(x, y, s=areas, marker='^',
c=colors, alpha=0.85)
#plt.scatter(x, y, s=areas, marker='o',
c=colors, alpha=0.85)
plt.axis([0.0, 1.0, 0.0, 1.0])
plt.savefig('3.png')
plt.show()
```

Overleaf and tikz

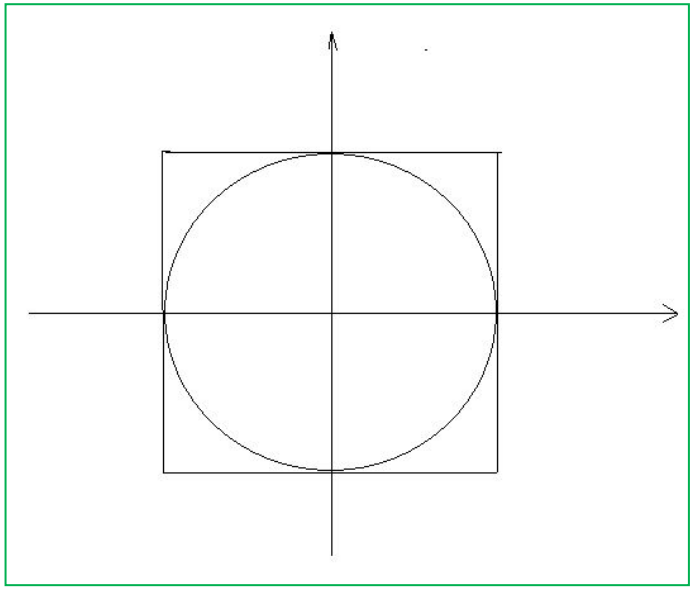
```
\documentclass{article}
\usepackage{tikz}
\usetikzlibrary{arrows,shapes,positioning}
\usetikzlibrary{decorations.markings}
\tikzstyle arrowstyle=[scale=1]
\tikzstyle directed=[postaction={decorate,decoration={markings,
    mark=at position .65 with {\arrow[arrowstyle]{stealth}}}}]
\tikzstyle reverse directed=[postaction={decorate,decoration={markings,
    mark=at position .65 with {\arrowreversed[arrowstyle]{stealth};}}}]

\begin{document}
\begin{tikzpicture}
\draw[gray, thick] (-5,0) -- (-0.3,0);
\node at ( -5,-0.3)    {-$L_l$};
\node at ( -0.6,-0.3)    {-$L_{0}$};
\node at ( 5,-0.3)    {+$L_l$};
\node at ( 0.6,-0.3)    {+$L_{0}$};
\draw[gray, ultra thick] (-3.3,0) -- (-2.8,0);
\filldraw [gray] (-5,0) circle (2pt);
\filldraw [gray] (-0.3,0) circle (2pt);
\node at ( -2.8,-0.2)    {$dx$};
\draw[blue,thick,directed] (-3.3,0) -- (0,2.5);
\draw[blue,thick,directed] (-2.8,0) -- (0,2.1);
\draw[blue,thick,directed] (-3.3,0) -- (0,-2.5);
\draw[blue,thick,directed] (-2.8,0) -- (0,-2.1);
\draw[gray, thick] (5,0) -- (0.3,0);
\filldraw [gray] (5,0) circle (2pt);
\filldraw [gray] (0.3,0) circle (2pt);
\node[] at (-2.2,0.2)  {$\theta$};
%\draw (-2.8,0) arc (0:30:1)
\draw[red,thick,directed] (3.3,0) -- (0,2.5);
\draw[red,thick,directed] (2.8,0) -- (0,2.1);
\draw[red,thick,directed] (3.3,0) -- (0,-2.5);
\draw[red,thick,directed] (2.8,0) -- (0,-2.1);

\fill[gray!50] (0,0) ellipse (0.2 and 4.);
\end{tikzpicture}
\end{document}
```





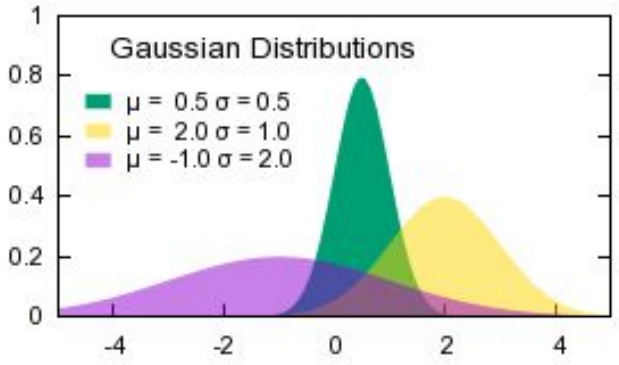
CERN Root例2：随机数计算Pi

```
void random()
{
//TRandom3, is based on the "Mersenne
Twister generator", and is the
recommended one, since it has good
random proprieties (period of about
10**6000 ) and it is fast
      // create random number generator
      gRandom = new TRandom3(0);
      gRandom2 = new TRandom3(1);
      int n=20000;
      int ftot=0;
      for (int i = 0; i < n; ++i) {
        double x=gRandom->Uniform(-1,1);
        double y=gRandom2->Uniform(-1,1);
        double r=sqrt(x*x+y*y);
        if(r<1.0) {ftot++;}
      }

     cout<<4*float(ftot)/float(n)<<endl;

}
```

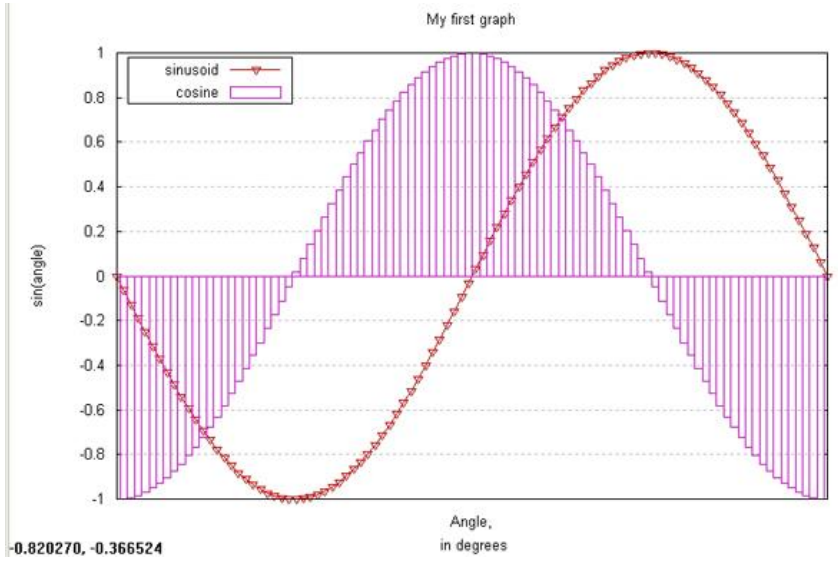


GNUPLOT

http://www.gnuplot.info/



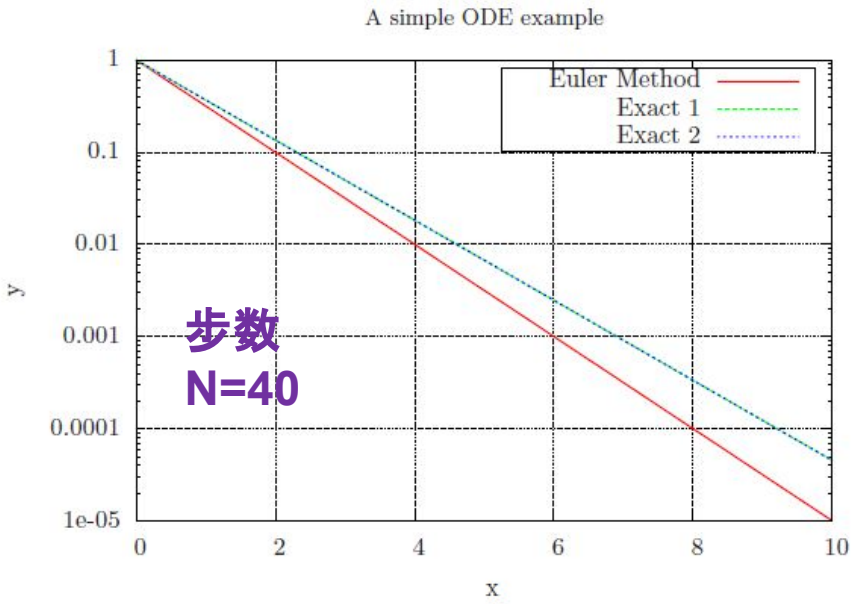
Gnuplot is a portable **command-line driven graphing utility** for Linux, OS/2, MS Windows, OSX, VMS, and many other platforms. The source code is copyrighted but freely distributed (i.e., you don't have to pay for it). It was **originally created to allow scientists and students to visualize** mathematical functions and data **interactively**, but has grown to support many non-interactive uses such as web scripting. It is also used as a plotting engine by third-party applications like Octave. Gnuplot has been supported and under active development since 1986.

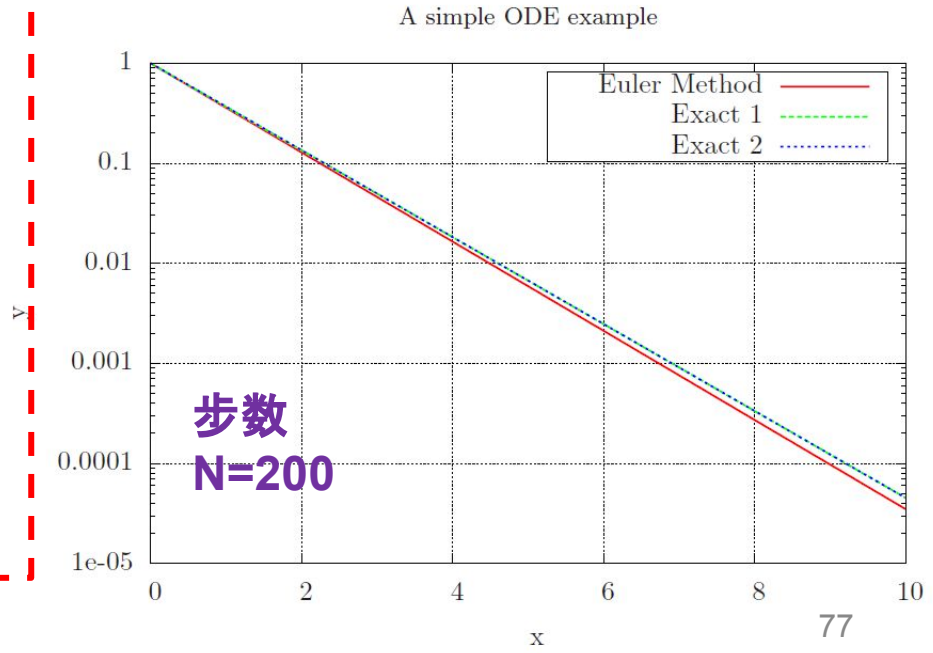


例：常微分方程求解

An ODE Example: $y' = -y$,
with y(0)=1. x:[0-10]
Explicit Method

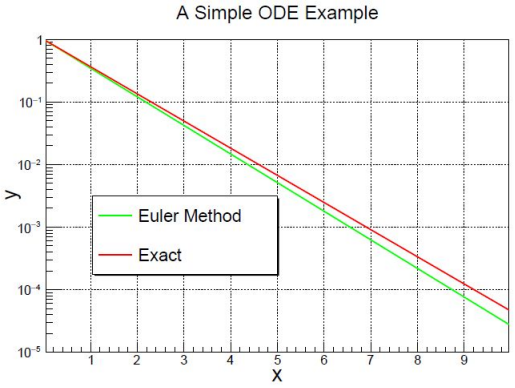
t	output	exact
0.0000000E+00	0.1000000E+01	0.1000000E+01
0.2000000E+00	0.8000000E+00	0.8187308E+00
0.4000000E+00	0.6400000E+00	0.6703200E+00
0.6000000E+00	0.5120000E+00	0.5488116E+00
0.8000000E+00	0.4096000E+00	0.4493290E+00
0.1000000E+01	0.3276800E+00	0.3678794E+00
……		
0.2000000E+01	0.1073742E+00	0.1353353E+00
……		
0.5000000E+01	0.3777893E-02	0.6737947E-02
0.8000000E+01	0.1329228E-03	0.3354626E-03
……		
0.9400000E+01	0.2787593E-04	0.8272407E-04
0.9600000E+01	0.2230075E-04	0.6772874E-04
0.9800000E+01	0.1784060E-04	0.5545160E-04
0.1000000E+02	0.1427248E-04	0.4539993E-04





例2：CERN ROOT作图

```
void rootplot()
{
   TCanvas *c1 = new
TCanvas("c1","",200,10,700,500);
   c1->SetGrid();

   Int_t n = 101;
   float Rbin[101],R2U[101],R2C[101];

   float xbin,xp,yp;
   int flag=0;
   int k0=0;
   int ka=0;
   int kb=0;
   FILE *fp = fopen("plot2.gnu","r");
   while (1) {
     flag=fscanf(fp,"%f %f %f",&xbin,&xp,&yp);
     if(flag!=3)break;
     Rbin[k0]=xbin;
     R2U[k0]=xp;
     R2C[k0]=yp;
     k0++;
   }
```

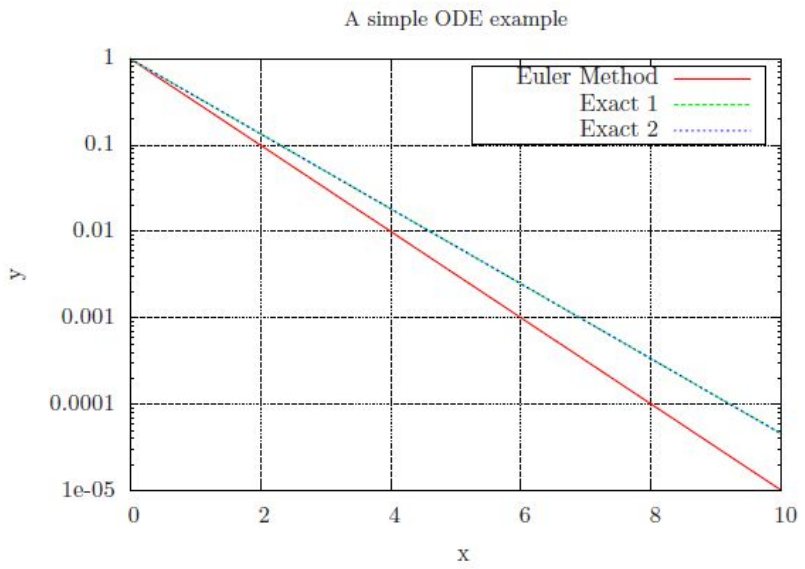



```
 TMultiGraph *mg = new TMultiGraph();
   mg->SetTitle("A Simple ODE Example; x; y");
   gr = new TGraph(n,Rbin,R2U);
   gr->SetLineWidth(2);
   gr->SetLineColor(3);
   gr2 = new TGraph(n,Rbin,R2C);
   gr2->SetLineWidth(2);
   gr2->SetLineColor(2);
   mg->Add(gr);
   mg->Add(gr2);
   mg->Draw("AC");
   mg->GetXaxis()->SetRangeUser(0.1,9.9);
   mg->GetYaxis()->SetRangeUser(0.00001,1.);
   mg->GetXaxis()->SetTitle("x");
   mg->GetXaxis()->SetTitleSize(.06);
   mg->GetYaxis()->SetTitle("y");
   mg->GetYaxis()->SetTitleSize(.06);
   mg->GetXaxis()->CenterTitle();
   mg->GetYaxis()->CenterTitle();
   mg->GetXaxis()->SetTitleOffset(0.6);
   mg->GetYaxis()->SetTitleOffset(0.6);
   c1->SetLogy();
   gPad->Modified();
   TLegend *l1 = new TLegend(0.18,0.3,0.5,0.5);
   l1->SetBorderSize(2);
   l1->SetFillColor(0);
   l1->AddEntry(gr,"Euler Method","l");
   l1->AddEntry(gr2,"Exact","l");
   l1->Draw();
   c1->SaveAs("example-N100-2.pdf");
}
```

例3：GNUPLOT作图

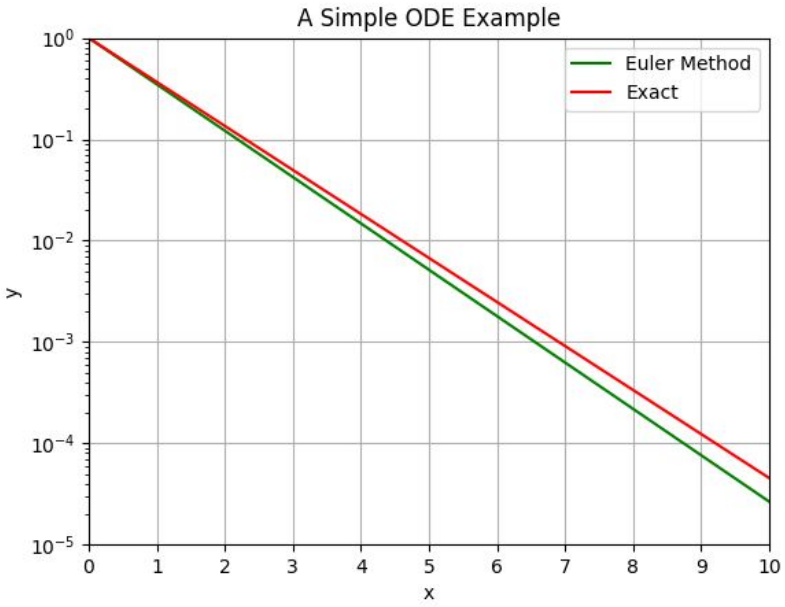
tot.tex

```
\documentclass[17pt]{article}
\usepackage{graphicx,color}
\begin{document}
\thispagestyle{empty}
\input{data.tex}
\end{document}
```




```
set pointsize 2.0
set tics in
set log y
set mytics 10
set grid
set xrange[0:10]
set terminal epslatex color
set output "data.tex"
set title '{\small A simple ODE example}'
set ylabel 'y'
set xlabel 'x'
set xlabel offset 0.5
set ylabel offset 2.5
set key box
plot "plot.gnu"   index 0 u ($1):($2)    title
'Euler Method' w l  lt 1 lw 3 ,\
    "plot.gnu"   index 0 u ($1):($3)    title
'Exact 1'              w l  lt 2 lw 3 ,\
    exp(-x)      title'Exact 2'   w l  lt 3  lw 3
set output
!latex tot.tex
!dvips -E tot.dvi -o example1.eps
!epstopdf example1.eps
```

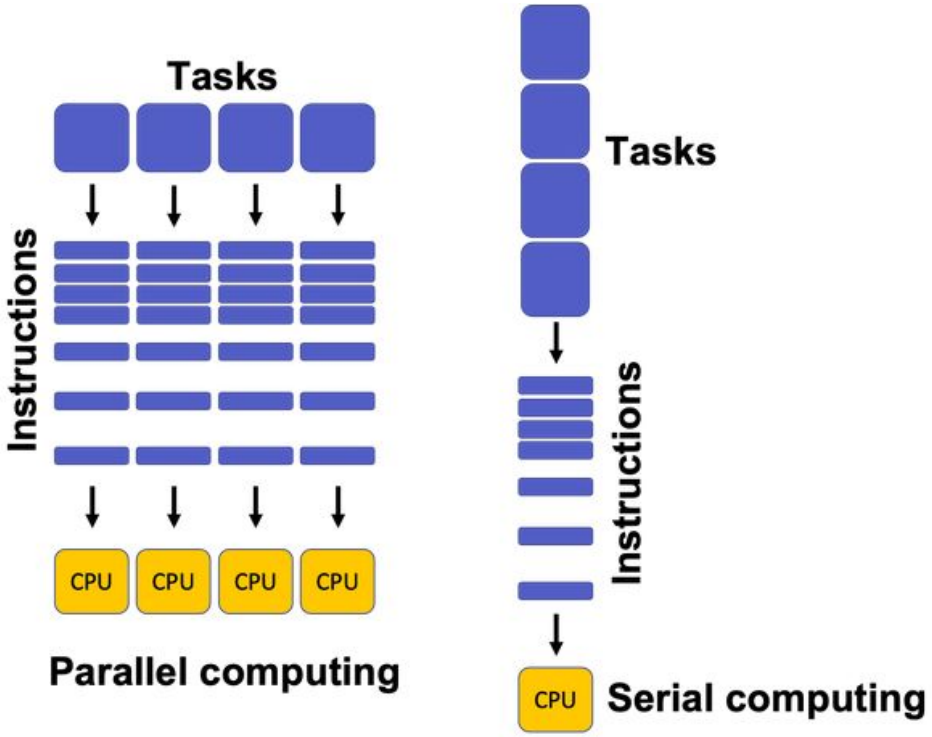
例3：Python作图




```
import matplotlib.pyplot as plt
import csv
import numpy as np

x = []
y = []
z = []
with open('plot.gnu','r') as csvfile:
    plots = csv.reader(csvfile, delimiter=' ',
skipinitialspace=True)
    for row in plots:
        print(row)
        x.append(float(row[0]))
        y.append(float(row[1]))
        z.append(float(row[2]))
plt.semilogy()
plt.xticks(np.arange(0, 11, 1))
plt.xlim(0, 10)
plt.ylim(0.00001, 1)
plt.plot(x,y, color='green', label='Euler Method')
plt.plot(x,z, color='red', label='Exact')
plt.grid()
plt.xlabel('x')
plt.ylabel('y')
plt.title('A Simple ODE Example')
plt.legend()
plt.savefig('4.png')
plt.show()
```

并行计算 Python

```
import multiprocessing as mp
print(f"Number of cpu: {mp.cpu_count()}")
```



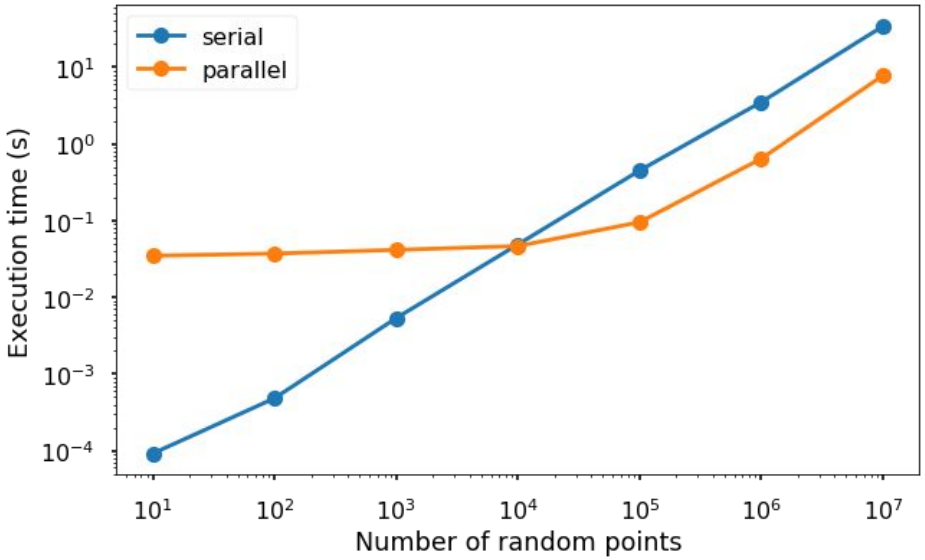
A **process** is an instance of a program (such as Python interpreter, Jupyter notebook etc.). A process is created by the operating system to run program, and each process has its own memory block.

A **thread** is a sub-process that reside within the process. Each process can have multiple threads, that these threads will share the same memory block within the process. Therefore, for multiple threads in a process, due to the shared memory space, the variables or objects are all shared.

并行计算 Python

```
import numpy as np
import time
def random_square(seed):
        np.random.seed(seed)
        random_num =
np.random.randint(0, 10)
        return random_num**2
t0 = time.time()
results = []
for i in range(10000000):
results.append(random_square(i))
t1 = time.time()
print(f'Execution time {t1 - t0} s')
```

```
import multiprocessing as mp
import numpy as np
import time
def random_square(seed):
        np.random.seed(seed)
        random_num = np.random.randint(0, 10)
        return random_num**2
t0 = time.time()
n_cpu = mp.cpu_count()
pool = mp.Pool(processes=n_cpu)
results = [pool.map(random_square,
range(10000000))]
t1 = time.time()
print(f'Execution time {t1 - t0} s')
```



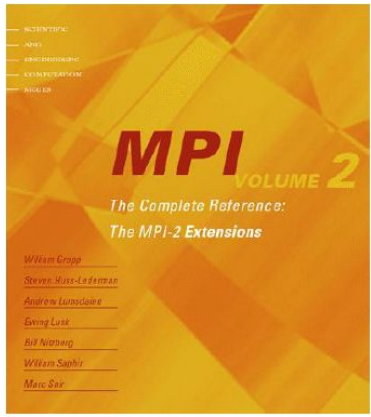
并行计算 MPI

Modern parallel programing: **open-MP** and **MPI**.
–Lots of processors connected and coordinating to solve large problems

M P I = Message Passing Interface.
https://www.mpi-forum.org/docs/
A standardized collection of routines (functions) which is implemented for each programing language (Fortran, C, C++, Python).
First standardized in 1994 (MPI-1.0) and second in 1997 (MPI-2.0) and (MPI-3.0) after 2012. Currently MPI-2.0 is most widely used.

The two most widely used implementations are

- MPICH http://www.mpich.org
- open-MPI http://www.open-mpi.org
  Python implementation mpi4py
  (Note that open-MPI has nothing to do with openMP)



并行计算 MPI

sudo apt-get install libcr-dev mpich2 mpich2-doc

mpic++ -o example example.c
mpirun -n 2 ./example

MPI include file

.
.
.

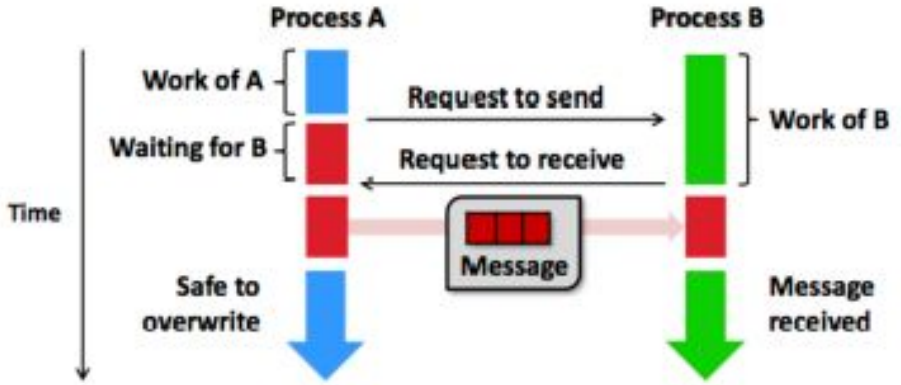
Initialize MPI environment

.
.
.

Do work and make message passing calls

.
.
.

Terminate MPI Environment



并行计算 MPI

```
#include <mpi.h>
#include <stdio.h>

int main(int argc, char ** argv)
{
    int rank, size;

    MPI_Init(&argc, &argv);

    MPI_Comm_rank(MPI_COMM_WORLD, &rank);
    MPI_Comm_size(MPI_COMM_WORLD, &size);
    printf("I am %d of %d\n", rank, size);

    MPI_Finalize();
    return 0;
}
```

Basic requirements for an MPI program

Data communication in MPI is like email exchange
–One process sends a copy of the data to another process (or a group of processes), and the other process receives it

并行计算 MPI

```
printf("For rank %d count = %d itrr = %d\n",rank,count,no_div);
MPI_Reduce(&count,&total_count,1,MPI_INT,MPI_SUM,0,MPI_COMM_WORLD);
MPI_Reduce(&no_div,&fin_no,1,MPI_INT,MPI_SUM,0,MPI_COMM_WORLD);
```

```
double t1, t2;
int rank,size,i;
double x=0,y=0,pi,z;
int no = atoi(argv[1]);
int count=0,total_count=0,no_div=0,fin_no = 0;
MPI_Init(&argc,&argv);
t1 = MPI_Wtime();
MPI_Comm_rank(MPI_COMM_WORLD,&rank);
MPI_Comm_size(MPI_COMM_WORLD,&size);
printf("rank= %i ; size= %i\n", rank, size);
no_div = no/size;
srand ( time(NULL) );
for(i=0;i<no_div;i++)
        {
        x=rand()/(double)RAND_MAX;
        y=rand()/(double)RAND_MAX;
        z=x*x+y*y;
        if(z<=1)
        count++;
        }
```

```
t2 = MPI_Wtime();
printf("total time for rank %i: = %lf\n", rank, t2-t1);

if(rank ==0){
printf("        \n");
printf("*** Average over all processors ***\n");
printf("Total count  = %d, total itrr = %d\n",total_count,fin_no);
pi = ((double)total_count)/fin_no*4.0000;
printf("Pi value = %lf\n",pi);
        }
MPI_Finalize();
```

并行计算 MPI

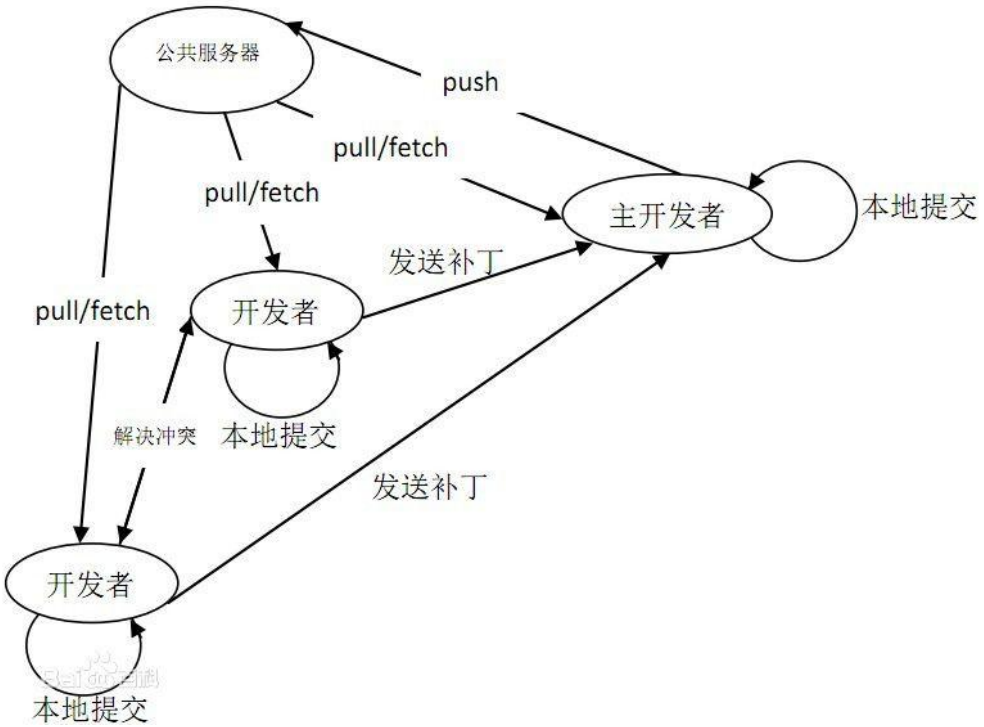
```
qliphy@qliphy-IdeaCentre-B520:~/Desktop/CP2019-new/MPI$ mpirun -n 1 ./pi 80000000
rank= 0 ; size= 1
For rank 0 count = 62831445 itrr = 80000000
total time for rank 0: = 1.796201

*** Average over all processors ***
Total count  = 62831445, total itrr = 80000000
Pi value = 3.141572
```

```
qliphy@qliphy-IdeaCentre-B520:~/Desktop/CP2019-new/MPI$ mpirun -n 4 ./pi 80000000
rank= 0 ; size= 4
rank= 1 ; size= 4
rank= 2 ; size= 4
rank= 3 ; size= 4
For rank 2 count = 15710006 itrr = 20000000
For rank 3 count = 15710006 itrr = 20000000
total time for rank 3: = 0.739523
total time for rank 2: = 0.739545
For rank 1 count = 15710006 itrr = 20000000
total time for rank 1: = 0.792446
For rank 0 count = 15710006 itrr = 20000000
total time for rank 0: = 0.816587

*** Average over all processors ***
Total count  = 62840024, total itrr = 80000000
Pi value = 3.142001
```

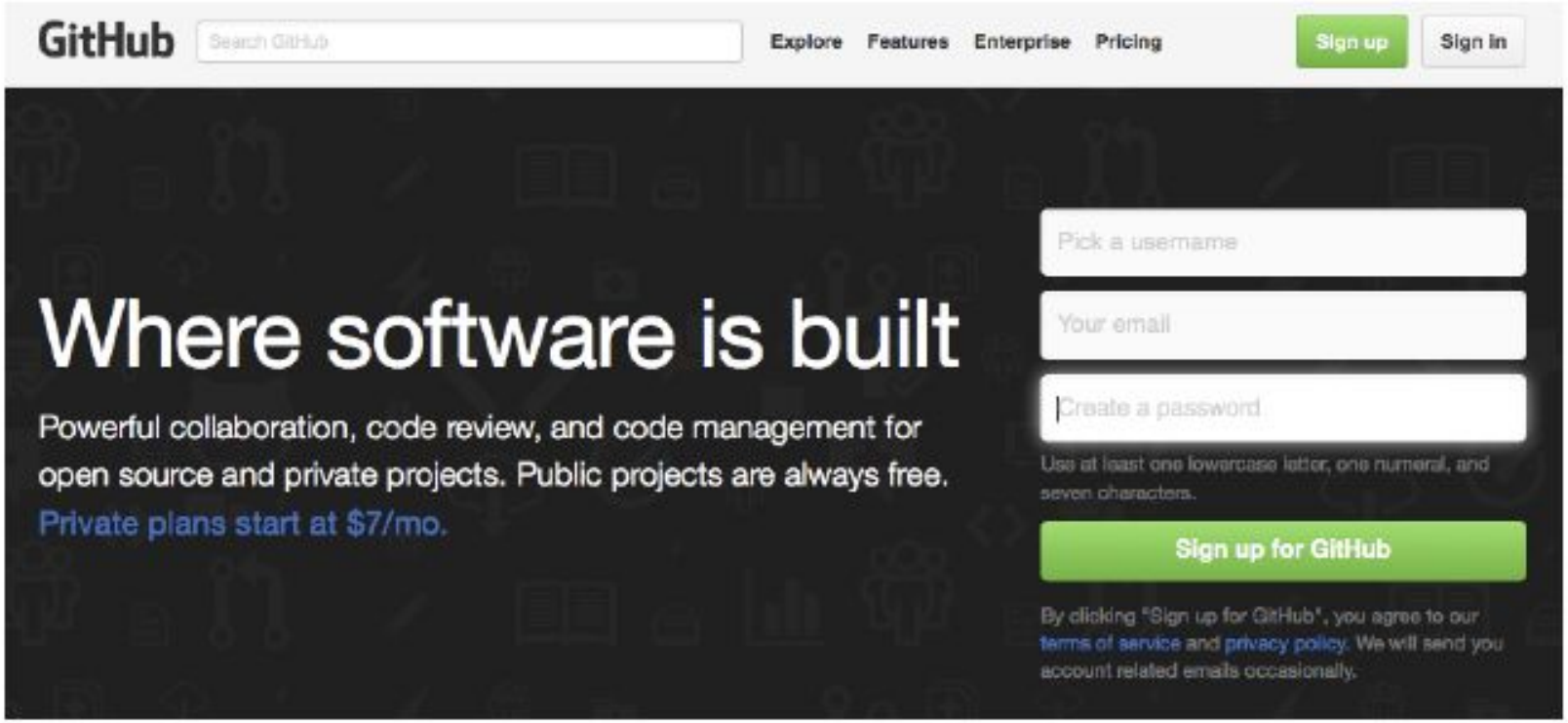
版本控制

- CVS (concurrent versions system)
- SVN (subversion)
- git

GitHub is a code hosting platform for version control and collaboration. It lets you and others work together on projects from anywhere.



Sign Up a Github Account



You will receive an activation email to confirm your email address

Set Up Git

https://help.github.com/articles/set-up-git/

1. Download and install the latest version of Git.

In terminal:

1. $ git config --global user.name "*YOUR NAME*”
2. $ git config --global user.email "*YOUR EMAIL ADDRESS*"

Authenticating with GitHub from Git

• Connecting over HTTPS (recommended)

If you clone with HTTPS, you can cache your GitHub password in Git using a credential helper.

https://help.github.com/articles/caching-your-github-password-ingit/

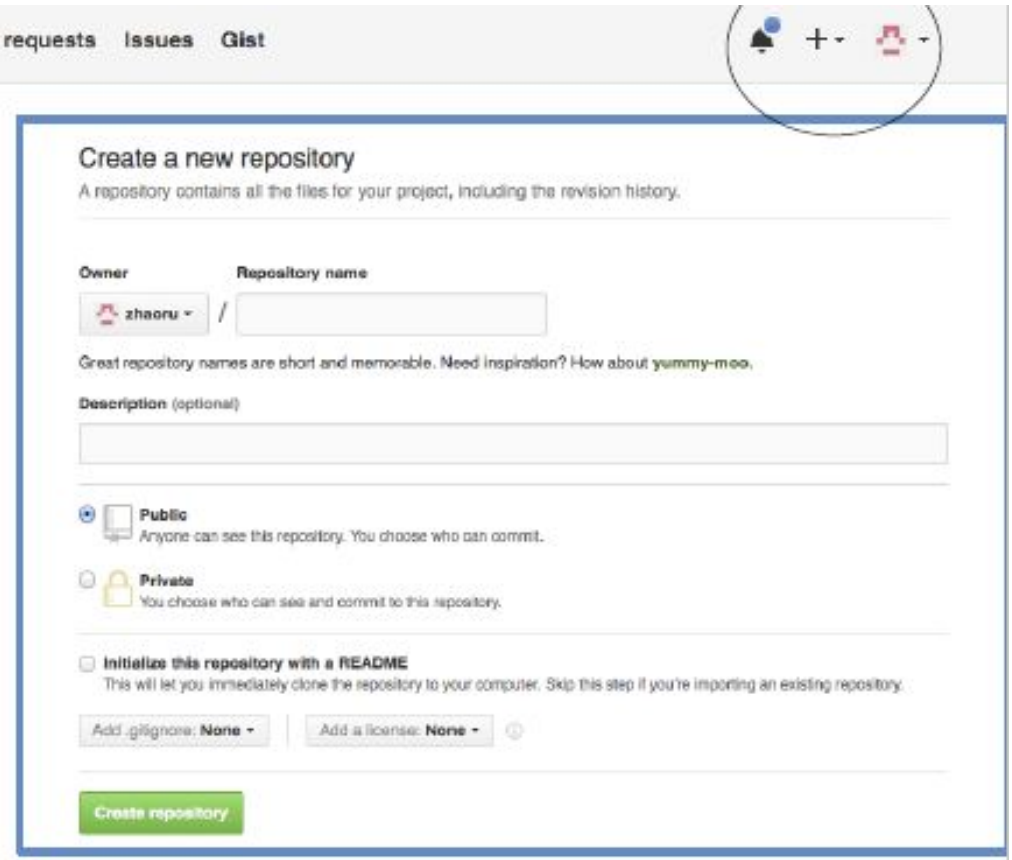
• Connecting over SSH

If you clone with SSH, you must generate SSH keys on each computer you use to push or pull from GitHub.

Create a Repo

https://help.github.com/articles/create-a-repo/

- Set up “Repo Name”
- Public
- **Don’t** select “Initialize this repository with a README ”
- Create Repository



Upload your file to the Repo

In terminal:

$ cd “target folder”

$ echo "# TEST4" >> README.md

$ git init

$ git add README.md

$ git add *

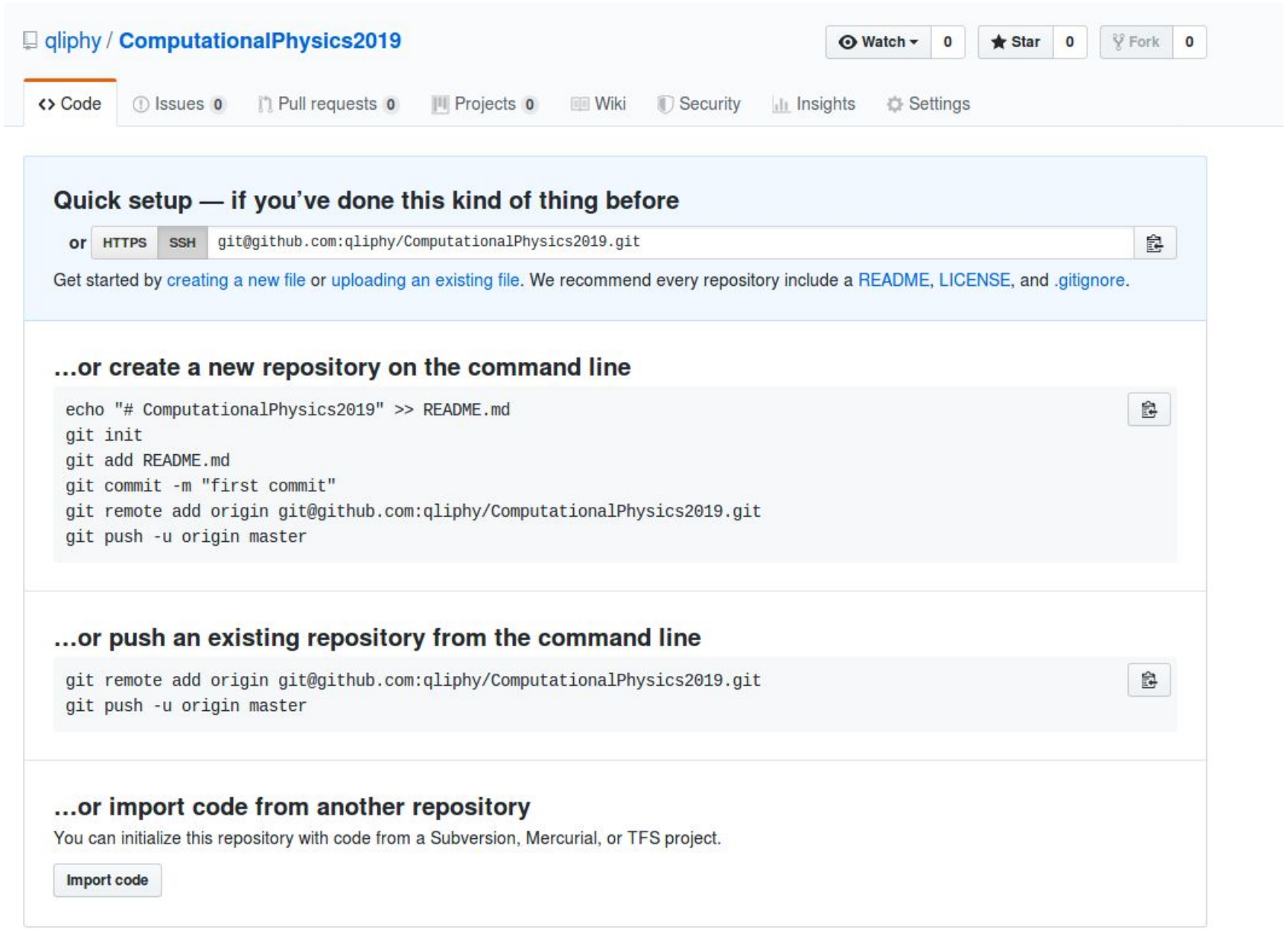
$ git commit -m "first commit"

$ git remote add origin git@github.com:XXX/TEST4.git (or https://)

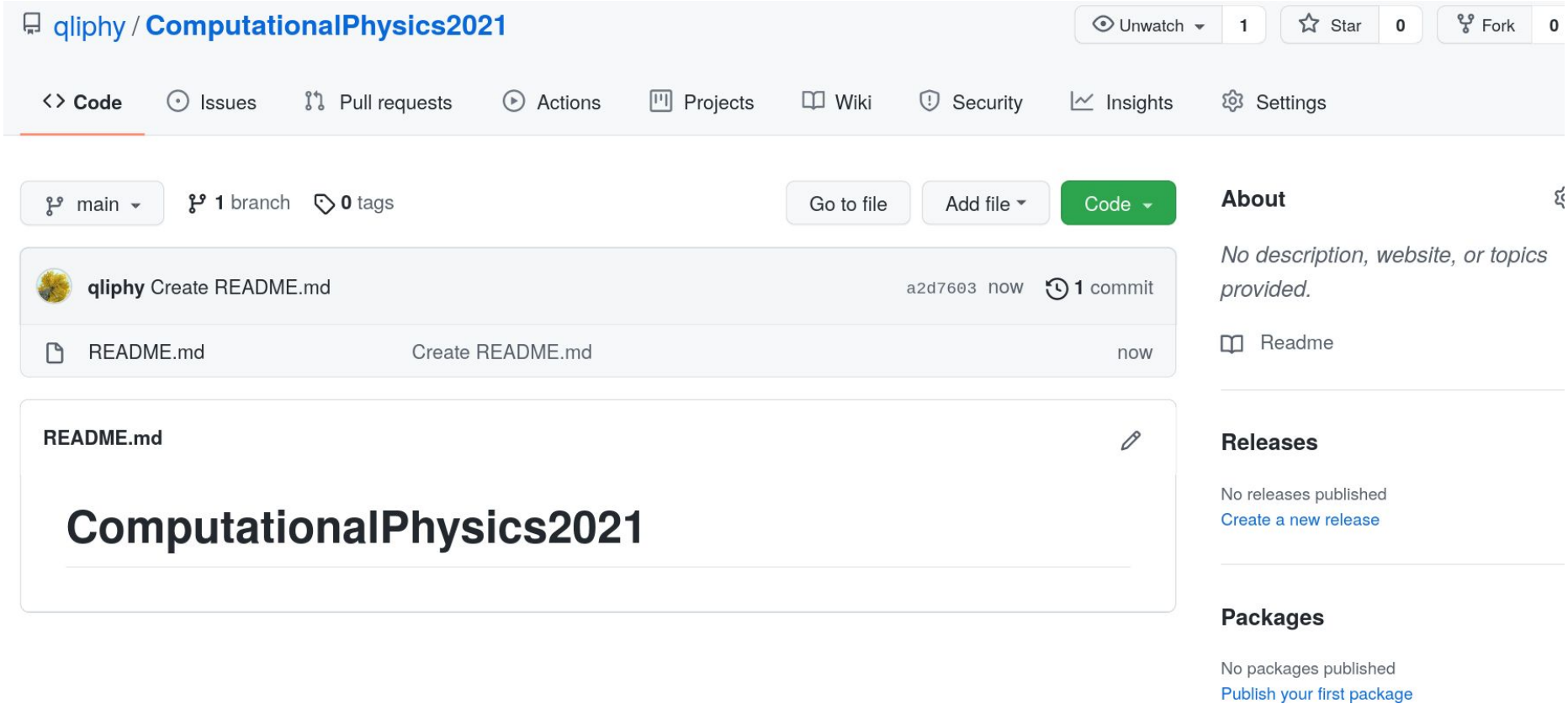
$ git push -u origin master

Then refresh your website. Upload successfully!

版本控制


qliphy / ComputationalPhysics2019
Watch 0
Star 0
Fork 0
Code
Issues 0
Pull requests 0
Projects 0
Wiki
Security
Insights
Settings
Quick setup — if you've done this kind of thing before
or HTTPS SSH git@github.com:qliphy/ComputationalPhysics2019.git
Get started by creating a new file or uploading an existing file. We recommend every repository include a README, LICENSE, and .gitignore.
...or create a new repository on the command line
echo "# ComputationalPhysics2019" >> README.md
git init
git add README.md
git commit -m "first commit"
git remote add origin git@github.com:qliphy/ComputationalPhysics2019.git
git push -u origin master
...or push an existing repository from the command line
git remote add origin git@github.com:qliphy/ComputationalPhysics2019.git
git push -u origin master
...or import code from another repository
You can initialize this repository with code from a Subversion, Mercurial, or TFS project.
Import code
ProTip! Use the URL for this page when adding GitHub as a remote.

版本控制



2021年的小作业：每位同学push一个以学号命名的文件夹到 XXX/ComputationalPhysics2021 @github