Physique numérique / *Computational Physics* (M1)

Supporting slides

Computational Physics

A — "Application of clever algorithms designed by *mathematicians* and *computer scientists,* in order to solve problems in physics for which we have already a good theoretical understanding — but we need the actual numbers for some predictions (the right prefactors, the right exponents, etc.)";

B — "A cheap way to do *experiments using a computer*, before actually doing them in the laboratory; a good way to estimate the most relevant parameters for a (costly) experiment";

C — "Something that *real* theoretical physicists would never do".

…

?

Timeline of scientific computing

From Wikipedia, the free encyclopedia

Before modern computers [edit]

18th century [edit]

- Simpson rediscovers Simpson rule, a century later.
- 1733 – The French naturalist Comte de Buffon poses his needle problem.[1][2]
- Euler comes up with a simple numerical method for integrands.[3][4][5]

19th century [edit]

- First formulation of Gram-Schmidt orthogonalisation by Laplace,[6] to be further improved decades later.[7][8][9][10]
- Babbage in 1822, began work on a machine made to compute/calculate values of polynomial functions automatically by using the method of finite differences. This was eventually called the Difference engine.
- Lovelace's note G on the Analytical Engine (1842) describes an algorithm for generating Bernoulli numbers. It is considered the first algorithm ever specifically tailored for implementation on a computer, and thus the first-ever computer programme.[11][12] The engine was never completed, however, so her code was never tested.[13]
- Adams-Bashforth method published.[14]
- In applied mathematics, Jacobi develops technique for solving numerical equations.[15][16][17]
- Gauss Seidel first published.
- To help with computing tides, Harmonic Analyser is built in 1886.

1900s (decade) [edit]

- 1900 – Runge's work followed by Martin Kutta to invent the Runge-Kutta method for approximating integration for differential equations.[18][19]

1910s (decade) [edit]

- 1910 – A-M Cholesky creates a matrix decomposition scheme.[20][21]
- Richardson extrapolation introduced.

1920s [edit]

- 1922 – Lewis Fry Richardson introduces numerical weather forecasting by manual calculation, using methods originally developed by Vilhelm Bjerknes as early as 1895.[22][23]
- 1926 – Grete Hermann publishes foundational paper for computer algebra, which established the existence of algorithms (including complexity bounds) for many of the basic problems of abstract algebra, such as ideal membership for polynomial rings.[24]
- 1926 Adams-Moulton method.
- 1927 – Douglas Hartree creates what is later known as the Hartree–Fock method, the first ab initio quantum chemistry methods. However, manual solutions of the Hartree–Fock equations for a medium-sized atom were laborious and small molecules required computational resources far beyond what was available before 1950.

Timeline of scientific computing

From Wikipedia, the free encyclopedia

physics !

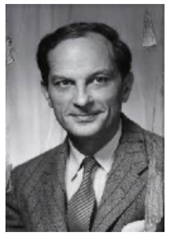
1930s [edit]

This decade marks the first major strides to a modern computer, and hence the start of the modern era.

- Fermi's Rome physics research group (informal name *I ragazzi di Via Panisperna*) develop statistical algorithms based on Comte de Buffon's work, that would later become the foundation of the Monte Carlo method. See also FERMIAC.
- Shannon explains how to use electric circuits to do Boolean algebra in "A Symbolic Analysis of Relay and Switching Circuits"
- John Vincent Atanasoff and Clifford Berry create the first electronic non-programmable, digital computing device, the Atanasoff–Berry Computer, from 1937-42.
- Complex number calculator created by Stibitz.

1940s [edit]

- 1947 – Monte Carlo simulation (voted one of the top 10 algorithms of the 20th century)[citation needed] invented at Los Alamos by von Neumann, Ulam and Metropolis.[25][26][27]
- George Dantzig introduces the simplex method (voted one of the top 10 algorithms of the 20th century)[citation needed] in 1947.[28]
- Ulam and von Neumann introduce the notion of cellular automata.[29]
- Turing formulated the LU decomposition method.[30]
- A. W. H. Phillips invents the MONIAC hydraulic computer at LSE, better known as "Phillips Hydraulic Computer".[31][32]
- First hydro simulations occurred at Los Alamos.[33][34]

1950s [edit]



- First successful weather predictions on a computer occurred.[35][36]
- Hestenes, Stiefel, and Lanczos, all from the Institute for Numerical Analysis at the National Bureau of Standards, initiate the development of Krylov subspace iteration methods.[37][38][39][40] Voted one of the top 10 algorithms of the 20th century.
- Equations of State Calculations by Fast Computing Machines introduces the Metropolis–Hastings algorithm.[41]
- Molecular dynamics invented by Bernie Alder and Wainwright [42][43]
- A S Householder invents his eponymous matrices and transformation method (voted one of the top 10 algorithms of the 20th century).[44]
- 1953 – Enrico Fermi, John Pasta, Stanislaw Ulam, and Mary Tsingou discover the Fermi–Pasta–Ulam–Tsingou problem through computer simulations of a vibrating string.[45]
- A team led by John Backus develops the FORTRAN compiler and programming language at IBM's research centre in San Jose, California. This sped the adoption of scientific programming,[46][47][48] and is one of the oldest extant programming languages, as well as one of the most popular in science and engineering.

STUDIES OF NON LINEAR PROBLEMS

E. FERMI, J. PASTA, and S. ULAM
Document LA-1940 (May 1955).

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

From the preface by S. Ulam

After the war, during one of his frequent summer visits to Los Alamos, Fermi became interested in the development and potentialities of the electronic computing machines. He held many discussions with me on the kind of future problems which could be studied through the use of such machines. We decided to try a selection of problems for heuristic work where in absence of closed analytic solutions experimental work on a computing machine would perhaps contribute to the understanding of properties of solutions. This could be particularly fruitful for problems involving the asymptotic—long time or "in the large" behavior of non-linear physical systems. In addition, such experiments on computing machines would have at least the virtue of having the postulates clearly stated. This is not always the case in an actual physical object or model where all the assumptions are not perhaps explicitly recognized.

Fermi expressed often a belief that future fundamental theories in physics may involve non-linear operators and equations, and that it would be useful to attempt practice in the mathematics needed for the understanding of non-linear systems. The plan was then to start with the possibly simplest such physical model and to study the results of the calculation of its long-time behavior. Then one would gradually increase the generality and the com-

Enrico Fermi

John Pasta

Stanislaw Ulam

Mary Tsingou

It should be stated here that during one summer Fermi learned very rapidly how to *program* problems for the electronic computers and he not only could plan the general outline and construct the so-called flow diagram but would work out himself the actual *coding* of the whole problem in detail.

feature article

Fermi, Pasta, Ulam, and a mysterious lady

Thierry Dauxois

PHYSICS TODAY

The computations for the first-ever numerical experiment were performed by a young woman named Mary Tsingou. After decades of omission, it is time to recognize her contribution.

Thierry Dauxois (thierry.dauxois@ens-lyon.fr) is a CNRS research director at École Normale Supérieure in Lyon, France.

Timeline of scientific computing

From Wikipedia, the free encyclopedia

1960s [edit]

- 1960 – First recorded use of the term "finite element method" by Ray Clough to describe the earlier methods of Richard Courant, Alexander Hrennikoff and Olgierd Zienkiewicz in structural analysis.[49]
- 1961 – John G.F. Francis[50][51] and Vera Kublanovskaya[52] invent QR factorization (voted one of the top 10 algorithms of the 20th century).
- 1963 – Edward Lorenz discovers the butterfly effect on a computer, attracting interest in chaos theory.[53]
- 1961 – Using computational investigations of the 3-body problem, Michael Minovitch formulates the gravity assist method.[54][55]
- 1964 – Molecular dynamics invented independently by Aneesur Rahman.[56]
- 1965 – fast Fourier transform developed by James W. Cooley and John W. Tukey.[57]
- 1964 – Walter Kohn, with Lu Jeu Sham and Pierre Hohenberg, instigates the development of density functional theory,[58][59] for which he shares the 1998 Nobel Chemistry Prize with John Pople.[60] This contribution is arguably the earliest work to which Nobels were given for a computer program or computational technique.
- First regression calculations in ecOnomics.

1970s [edit]

- 1975 – Benoit Mandelbrot coins the term "fractal" to describe the self-similarity found in the Fatou, Julia and Mandelbrot sets. Fractals become the first mathematical visualization tool extensively explored with computing.[61]
- 1977 – Kenneth Appel and Wolfgang Haken prove the four colour theorem, the first theorem to be proved by computer.[62][63][64]

1980s [edit]

- Fast multipole method (voted one of the top 10 algorithms of the 20th century) invented by Vladimir Rokhlin and Leslie Greengard.[65][66][67]
- Car–Parrinello molecular dynamics developed by Roberto Car and Michele Parrinello

1990s [edit]

- 1990 – In computational genomics and sequence analysis, the Human Genome Project, an endeavour to sequence the entire human genome, begins.
- 1998 – Kepler conjecture is almost all but certainly proved algorithmically by Thomas Hales.
- The appearance of the first research grids using volunteer computing – GIMPS (1996), distributed.net (1997) and Seti@Home (1999).

Download PDF | Generate Citation

Guest Editors' Introduction: The Top 10 Algorithms *(of the 20th Century)*

January/February 2000, pp. 22-23, vol. 2
DOI Bookmark: 10.1109/MCISE.2000.814652

Authors

Jack Dongarra
Francis Sullivan

invented by physicists

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

Physics is a fundamental driving force of scientific computing

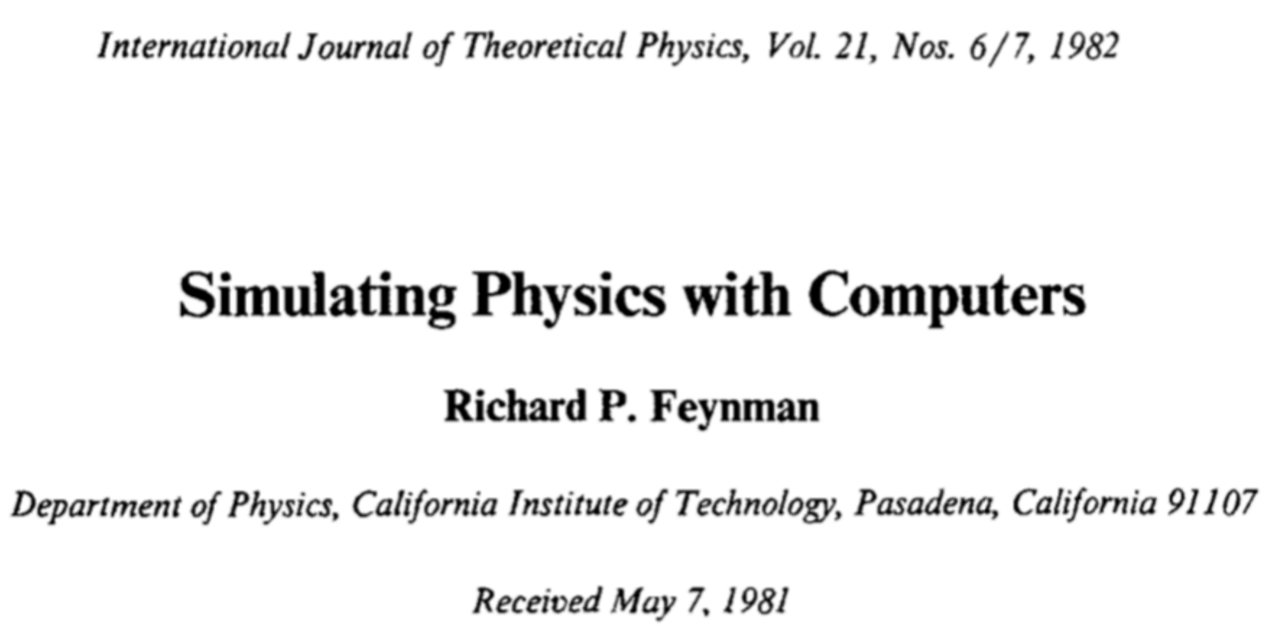
Physics & Computers

— Some of the *hardest computational problems* known in science are *raised by physics*;

— Some of the *hardest problems in physics* today are *computational problems*;

— Currently, **our understanding of the physical world is fundamentally limited by our computational capabilities** (both in terms of *software* as well as *hardware*);

— The interface between physics & computer science is generating lots of exciting developments (for *both* fields)
ex. quantum computing / quantum information

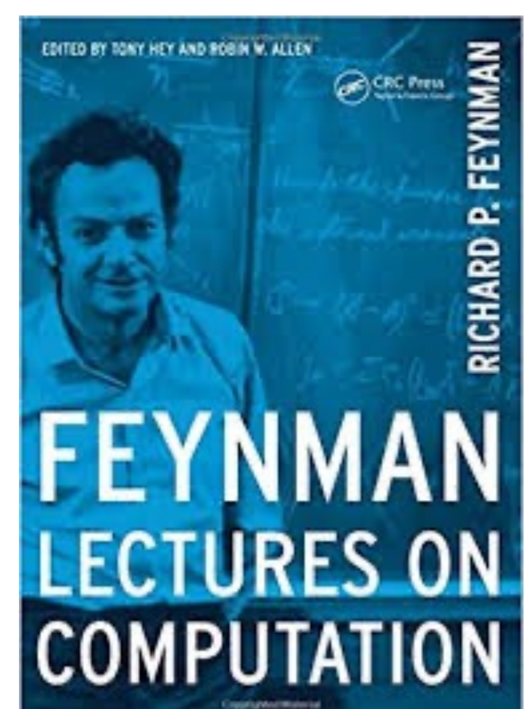

International Journal of Theoretical Physics, Vol. 21, Nos. 6/7, 1982

Simulating Physics with Computers

Richard P. Feynman

Department of Physics, California Institute of Technology, Pasadena, California 91107

Received May 7, 1981



Computational Physics

Physics & computation: a few milestones

“The book of nature is written in mathematical language”
«La filosofia [della natura] è scritta in questo grandissimo libro
che continuamente ci sta aperto dinanzi a gli occhi (io dico l’universo),
ma non si può intendere se prima non s’impara a intender la lingua,
e conoscere i caratteri ne’ quali è scritto.
Egli è scritto in lingua matematica…”
G. Galilei, *Il Saggiatore* (1623)

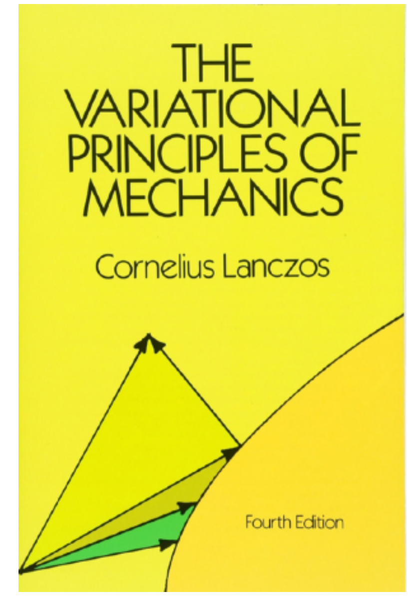
Could all physical problems be exactly solved *analytically*? NO
If this were true, the universe we live in would be a very different place
(no thermodynamics and statistical mechanics, etc.)

Physical (strong) Church-Turing thesis (simplified)
“Any physical system can be simulated by a Turing machine in polynomial time”

Quantum Church-Turing thesis (simplified)
“Any physical system can be simulated by a <u>quantum computer</u> in polynomial time”

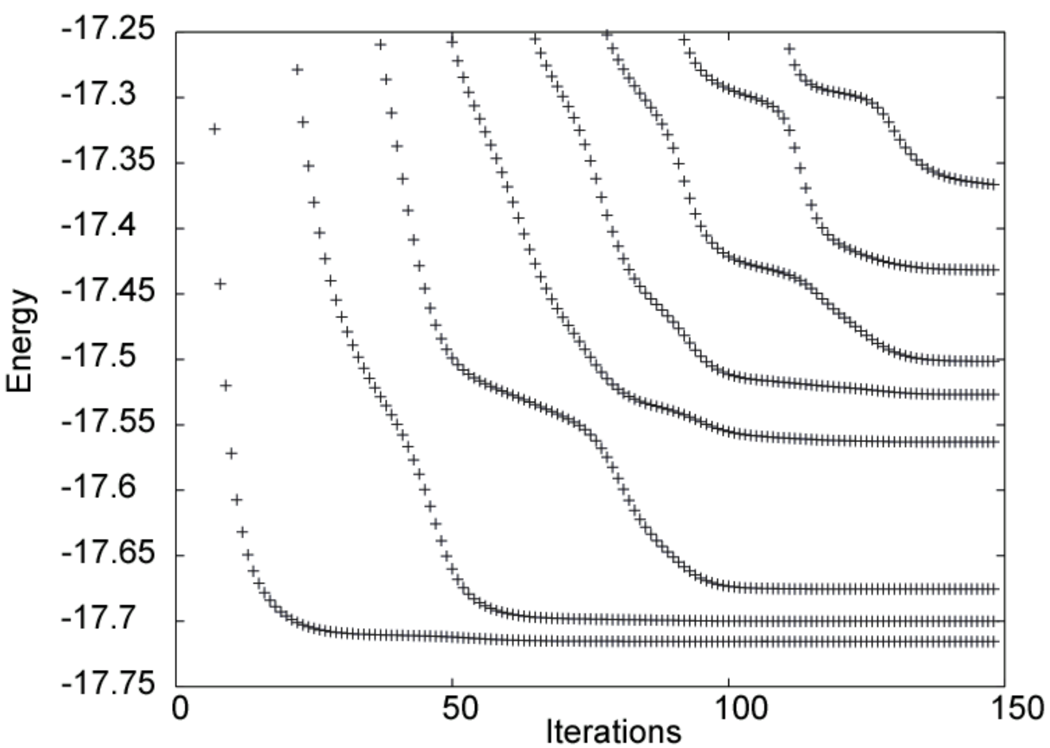
Lanczos algorithm

Cornelius Lanczos
(Lánczos Kornél)
one of the Martians…



Was du ererbt von deinen Vätern hast,
Erwirb es, um es zu besitzen.
GOETHE

DEDICATED
TO
ALBERT EINSTEIN



exponential convergence

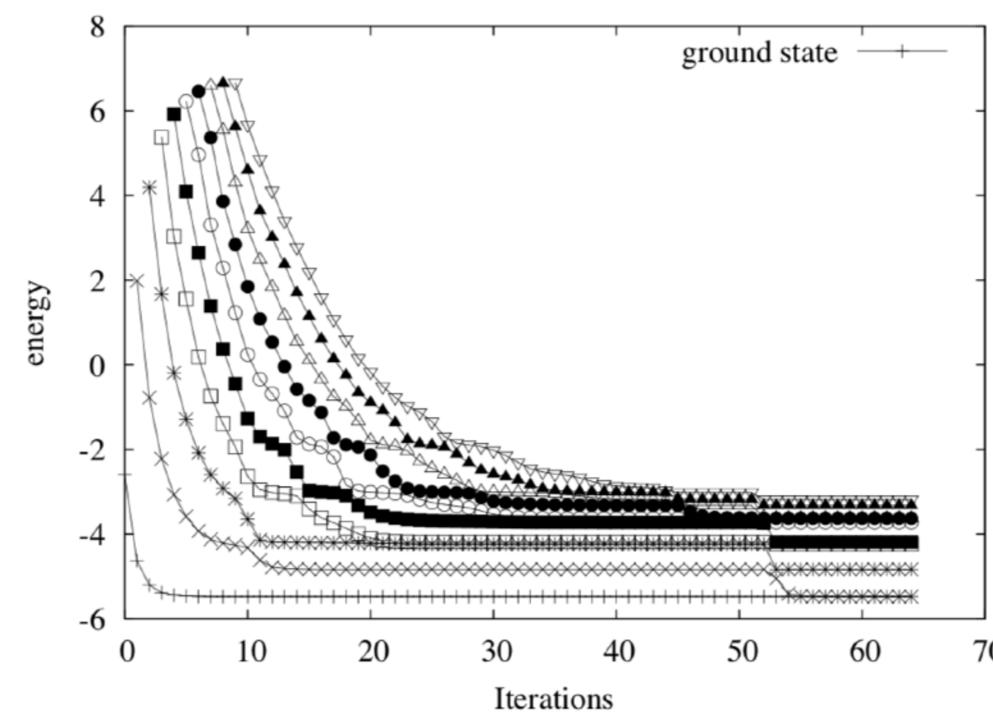
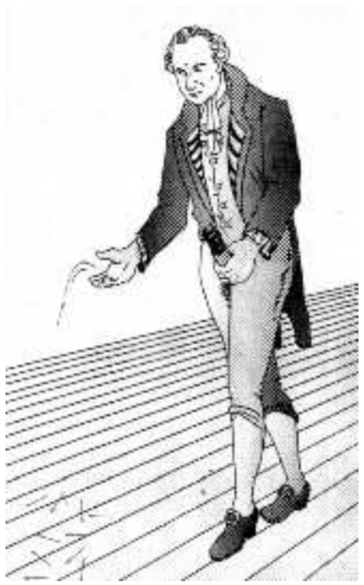


FIGURE 4. Typical convergence behavior of the Lanczos algorithm. In this example, convergence to the ground-state is already reached after approximately 10 iterations, while additional iterations are required to reach convergence for the excited states. "Ghost" eigenvalues appear and converge to a real eigenvalue as additional iterations are performed, leading to erroneous multiplicity at the completion of the calculation.

R. M. Noack and S. Manmana, arXiv:cond-mat/0510321

Origins of the Monte Carlo method

— Buffon's needle experiment



Georges-Louis Leclerc, Comte de Buffon (1707-1788)

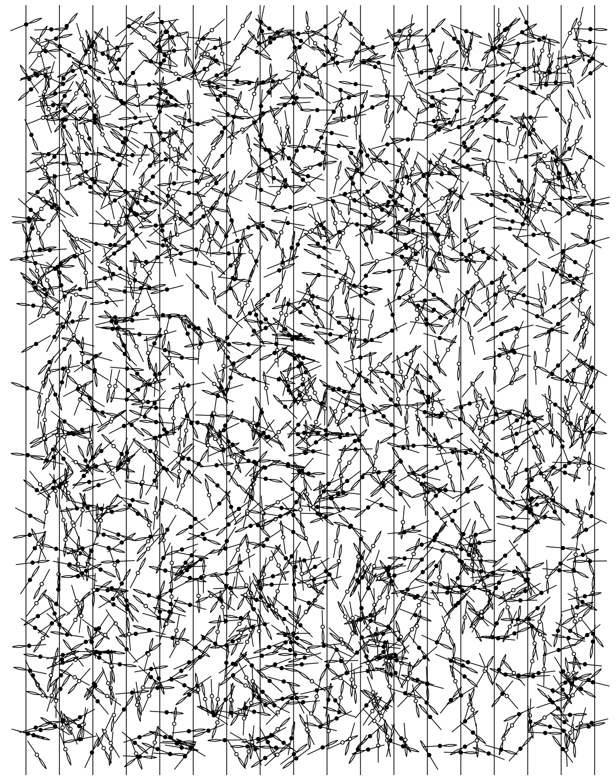
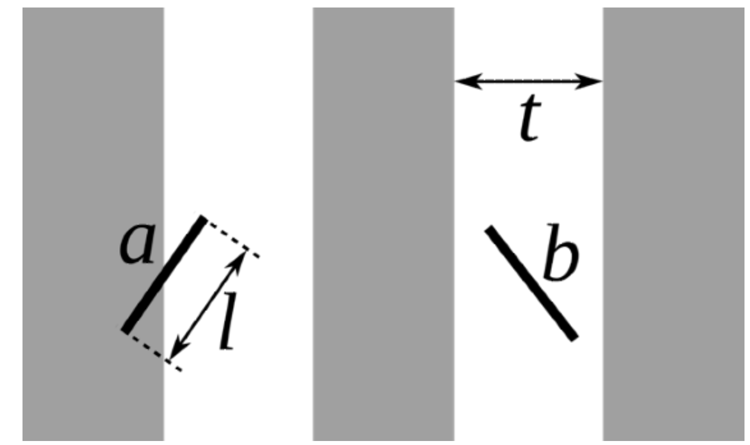


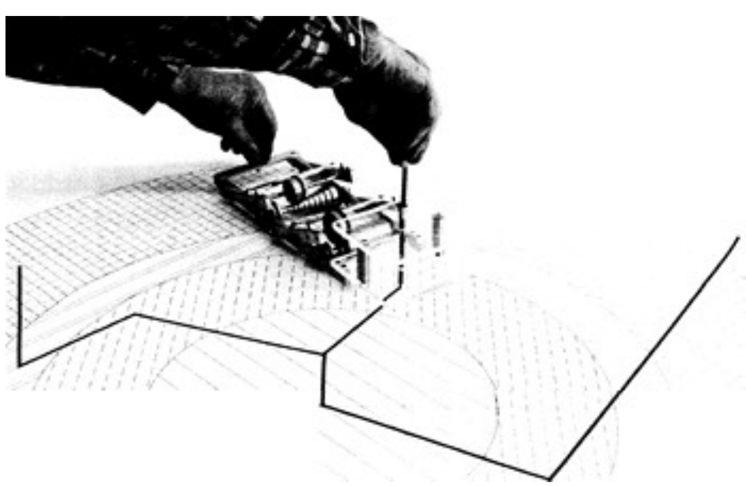
Fig. 1.10 Buffon's experiment with 2000 needles ($a = b$).



$$p = \frac{2}{\pi}\frac{l}{t}$$

probability that a needle falls across two bars (a)

— Fermi's FERMIAC (1930's)



study of propagation of neutrons through materials as a "random walk"