PHYD57 – Advanced Computations in Physical Sci.

LECTURE 1

- Structure of the course
- The 3rd Science: Computing.
- Motivational examples: astrophysics, neural computation
- History of early computing
- History of modern scientific computing
- Languages of High Perf. Computing

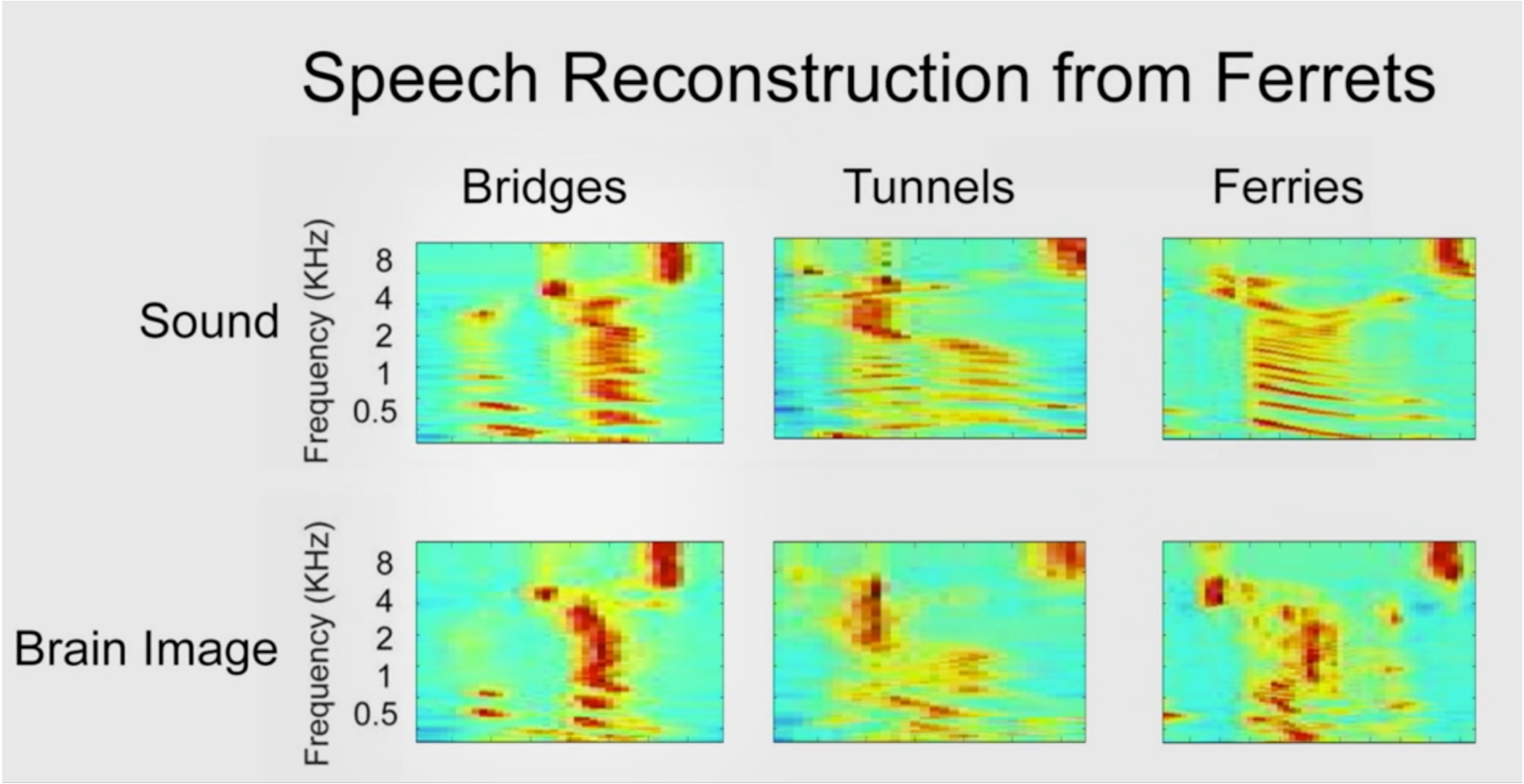
Literature

1. Paul Ceruzzi "A history of modern computing", 2nd ed., MIT Press 2003
2. http://computerhistory.org - Computer History Museum online
3. Norbert Schorghofer "Lessons in Scientific Computing" (2019)
5. Joshua Izaac & Jingbo Wang, "Computational Quant. Mech.", Springer (2018) – chapters on Python, Fortran

Apart from amazing physical simulations of the early Universe and other physical systems, computational science reaches much wider areas. For instance:
Is that a fact that animals can only make out some words we speak (or none at all)?

Not really. Animals are hearing very precisely all the phonemes we produce. And now we can reconstruct what they hear!

Ferret's electrical brain activity is decoded into audible sounds by a computer program (similar to convolutional neural net; we will return to this later in the course). The generated sounds are very similar to the experimenter's words. https://vimeo.com/42863899 (5:00)



ARCHIMEDES and the first computer

In 3rd century BC, the most famous scientist of antiquity **Archimedes (Ἀρχῑμήδης, 287-212 BC)** lived in one of the largest cities in the world - Syracuse, a Greek colony in eastern Sicily (now Italy).
Archimedes was a famous mathematician and physicist, also applied physicist (engineer) tasked by kings Hiero and Hieronymus to defend Syracuse with his mechanical contraptions shown below, during the Roman siege of Syracuse. Romans have won & Archimedes was killed, allegedly while drawing circles in the sand (although it may be a legend). A soldier of general Marcellus for some reason got angry and did not follow explicit orders to capture Archimedes alive.

ARCHIMEDES PALIMSEST

palimpsest = parchment (calve skin) which has been rubbed/erased to make space for a new text (e.g., Middle Age prayer book)

Fields Institute (UofT) awards medals equivalent to math Nobel prize with a (fake) picture of Archimedes.

Archimedes created the first laws of mechanics, such as the law of the lever, which also governs pulleys, buoyancy etc. In mathematics, until recently he was celebrated for his calculation of the area of circle, area under the parabola, area and volume of the sphere and the ratio of volumes of a cylinder and an inscribed sphere.

In a most interesting recent investigation, we found out from a previously lost book (Codex C or Archimedes' Palimpsest) that he understood and used infinity and infinitesimals, rediscovered after 1000+ years. Essentially, Archimedes was using integral calculus (Riemann integral) to derive areas and volumes.

ARCHIMEDES PALIMSEST

- before 213 BCE: Archimedes writes the treatise
- in 10th century CE, monks copy his original treatise
- in 1229 owner erases and recycles it as valuable parchment
- Palimpsest gets deposited in Metochion, Greek library in Constantinople (now Istanbul, Turkey) for many centuries
- in 1840s, German historian removes and published 1 page of math text
- in 1906, Danish historian Johan L. Heiberg examines the 174-page book after suspecting correctly that it's a treasure. The book is still in decent shape.

ARCHIMEDES' PALIMSEST

- In 1920s, the book disappears from Constantinople, re-surfaces in Paris
- The book disappears again, gets "augmented" by falsified drawings to increase its value (during WWII)
- Stored inappropriately, it decays from the relatively good state it was in 1906, due to mold etc.
- Palimpsest is sold at Sotheby's auction in London in 1998 for $2 mil to an anonymous buyer, who lets Walters Art Gallery staff (Baltimore, Md) and international experts restore and decipher *The Method of Mechanical Theorems* and other treatises, previously assumed lost.

ANTIKYTHERA MECHANISM = ancient analog/digital computer from The 2nd century BC.

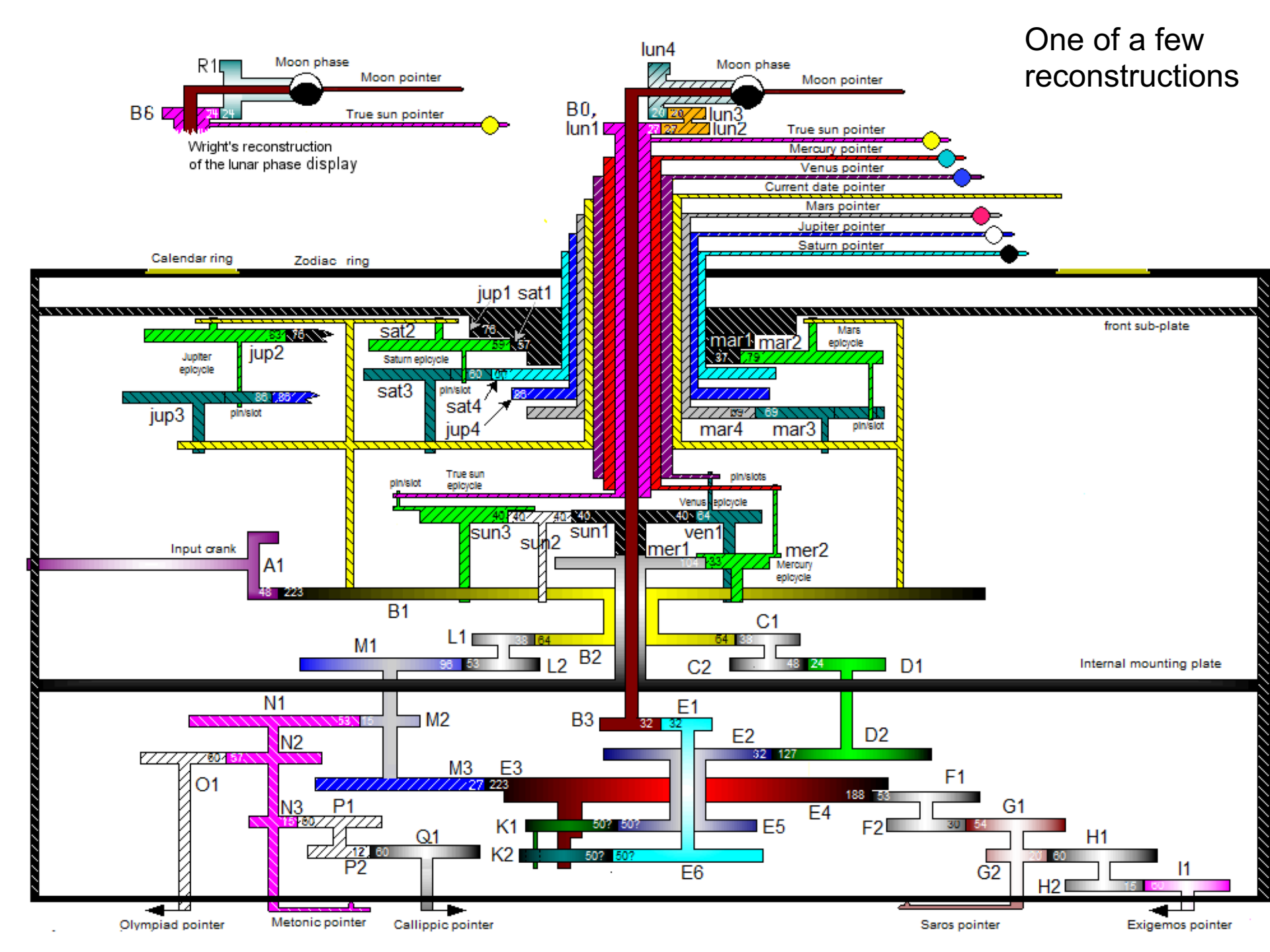
ANTIKYTHERA MECHANISM

Wiki page https://en.wikipedia.org/wiki/Antikythera_mechanism
and a video on youtube (below) desrcibe the finding of a mysterious mechanism in an ancient shipwreck on Greek island of Antikythera, as well as the international investigation that found by 3D X-ray scans technique how it functioned.

https://www.youtube.com/watch?v=jSQNEPbQOiI
(see around 17:20, 20:00, 40:00 min.)

The **Antikythera mechanism –** short video of reconstructed device
https://youtu.be/ZrfMFhrgOFc?t=163

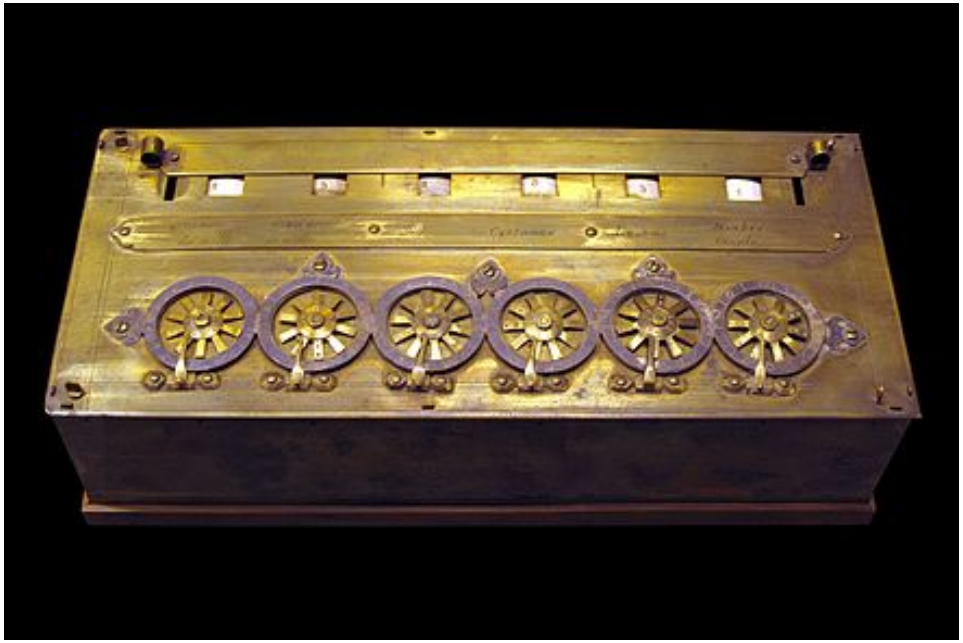
The mechanism is a partly digital (whole numbers of teeth on wheels reproduce rational numbers exactly) computer. Eccentric mounting of some parts reproduces in an analog form the non-uniform motion of the Moon). Analog value can be an arbitrary real number, as opposed to integer or a fraction.
It is the first known special-purpose mechanical computer of large complexity, only reached again by watchmakers in 1400s, that is 1.5k yrs later.

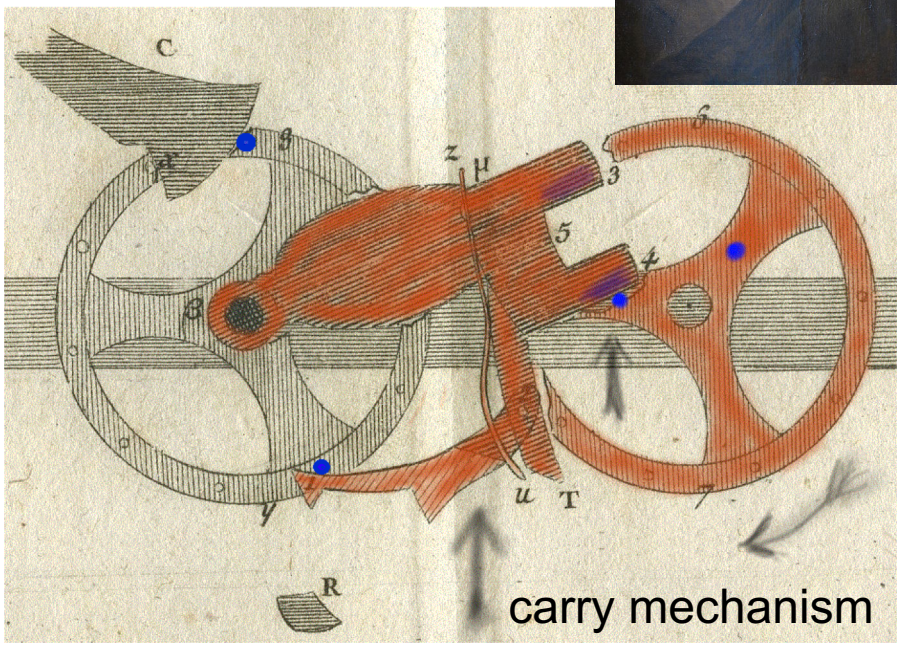

One of a few reconstructions
R1
Moon phase
Moon pointer
B6
True sun pointer
Wright's reconstruction of the lunar phase display
lun4
Moon phase
Moon pointer
B0, lun1
lun3
lun2
True sun pointer
Mercury pointer
Venus pointer
Current date pointer
Mars pointer
Jupiter pointer
Saturn pointer
Calendar ring
Zodiac ring
jup1 sat1
front sub-plate
sat2
jup2
Jupiter epicycle
Saturn epicycle
sat3
pin/slot
sat4
jup4
jup3
pin/slot
mar1
mar2
Mars epicycle
mar4
mar3
pin/slot
pin/slot
True sun epicycle
pin/slots
Venus epicycle
sun3
sun2
sun1
ven1
mer1
mer2
Mercury epicycle
Input crank
A1
B1
C1
M1
L1
L2
B2
C2
D1
Internal mounting plate
N1
M2
B3
E1
E2
D2
N2
O1
M3
E3
F1
E4
N3
P1
K1
E5
G1
F2
Q1
K2
H1
P2
E6
G2
I1
H2
Olympiad pointer
Metonic pointer
Callippic pointer
Saros pointer
Exigemos pointer

Willhelm Schickard - astronomer

In 1623 writes to Johannes Kepler about his 4-operation calculator using 6-digit numbers.
It is thought that larger number of wheels was prevented by mechanical friction problem.
Motivation to build:
astronomical table calculation.

Blaise Pascal (1623-1662) - physics & math prodigy, built adders/subtractors (calculators doing + and - operations)
Motivation: to mechanize tax collector's job.



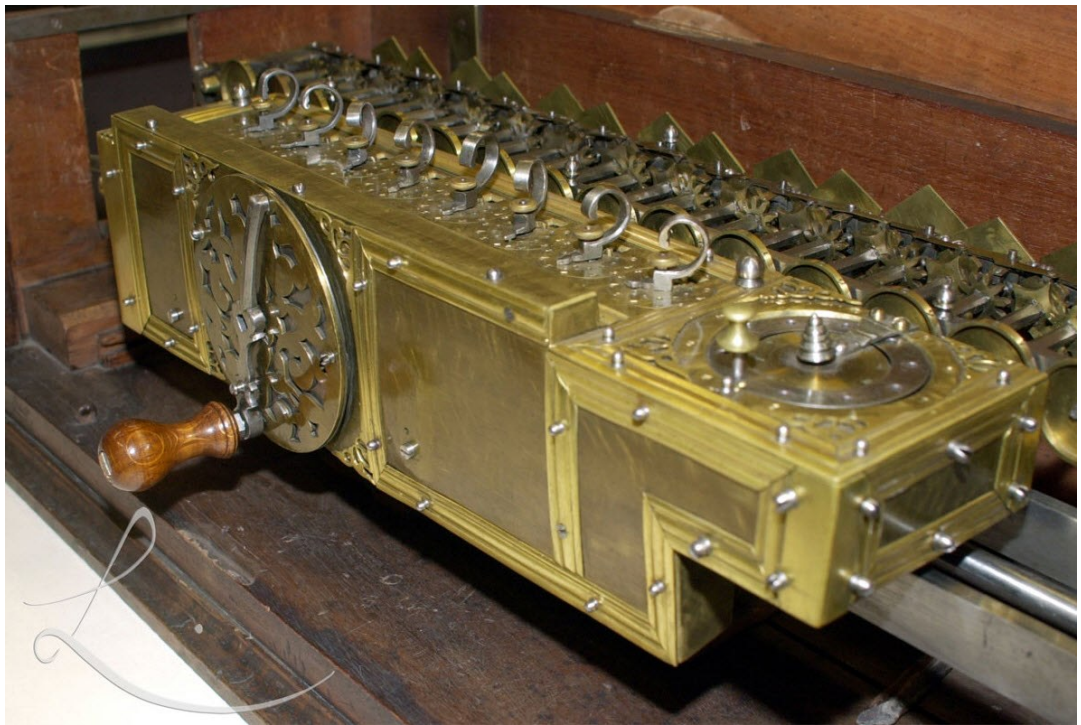


carry mechanism

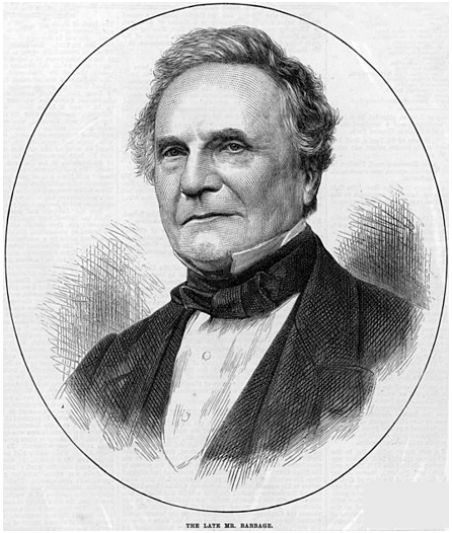
Gottfried Willhelm Leibnitz (1646-1716)

Invented calculus independently of Newton & published it first.
For example, *dy/dt* is Leibnitz notation (Newton used a dot over y)
One of his results:
$\pi = 4\ (1 - 1/3 + 1/5 - 1/7 + \ldots)$

Leibnitz developed the properties and use of the binary numbers (base-2 representation).
In 1675 Leibnitz built a digital mechanical calculator called "stepped reckoner", the first surviving 4-op. calculator (+ - * /)



Charles Babbage (1791- 1871)



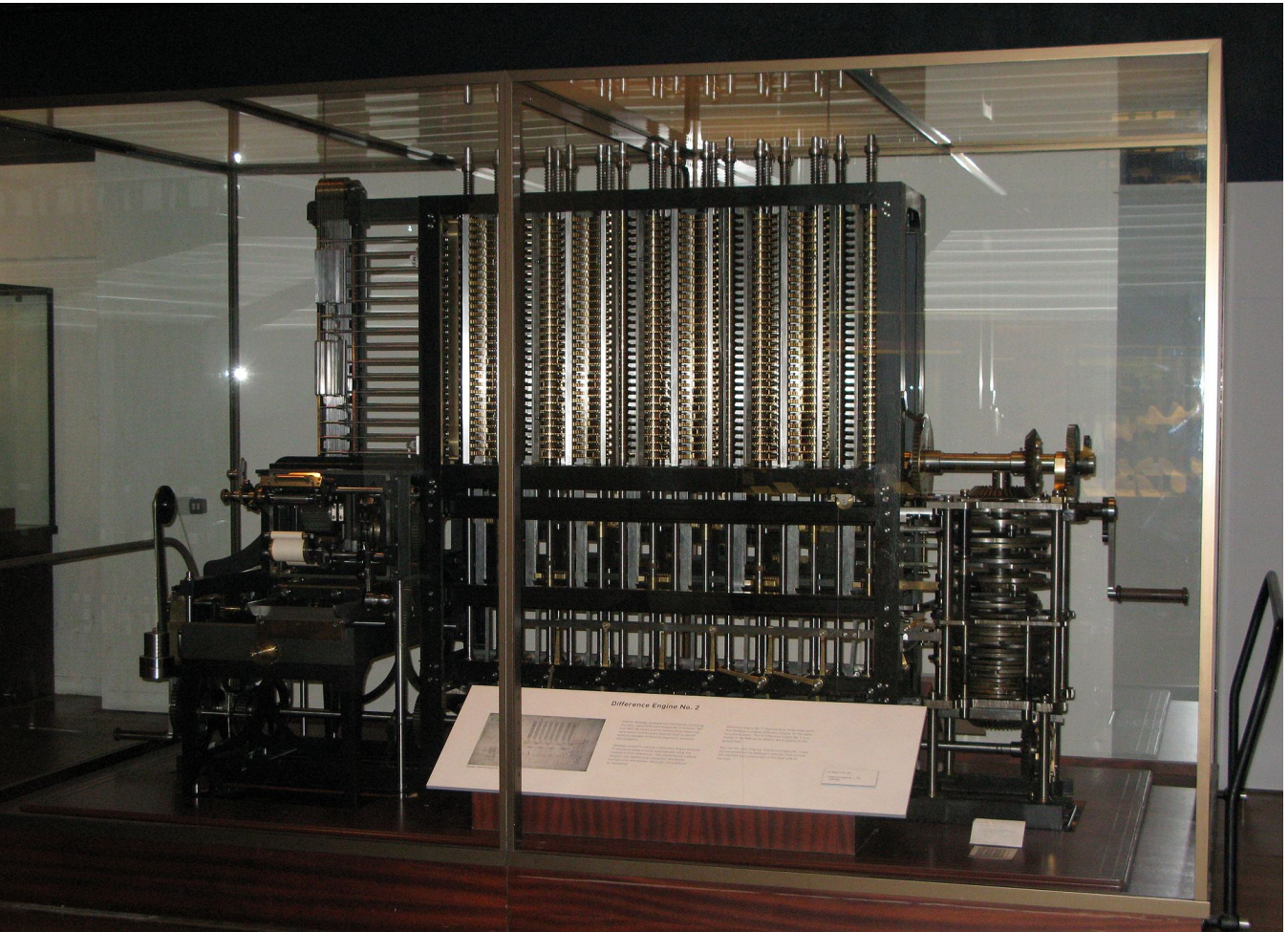
- Co-founded the Royal Astronomical Society
- 1812 - with Herschel recalculates The Nautical Almanac tables, finds errors.
- Becomes Lucasian Prof. of Mathematics at Cambridge, but not good at teaching
- Did operational research (division of labor etc.), cryptography, mechanical patents
- Inspired by French gov. project where mathematicians coordinated the effort of 80 human computers trained for specific sub-tasks, Babbage becomes convinced that a machine would be better than human at computation.

- Motivation: calculating mathematical and astronomical tables
- In 1823 Babbage obtained a grant to do mechanical calculation of tables, i.e. for the mechanical *computer* [until then and often for another 100 years, computer meant a person doing calculation]
- called the project "Differential Engine"
- method: finite differences to produce tables of polynomials of order up to 6 or 7

Charles Babbage (cont.)

- 1824 – medal of Royal Society for invention of “An engine to calculate mathematical and astronomical tables”,
- https://www.youtube.com/watch?v=be1EM3gQkAY (2012 video on reconstruction)
- The project was partially successful, but unfinished.

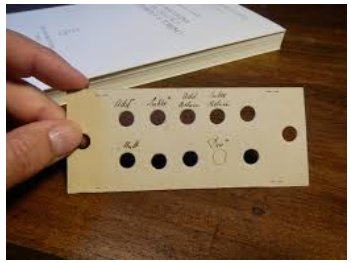
8000 parts,
5 tons, hand-cranked



Difference Engine no.2
(2008 reconstruction
from unrealized plans)

Charles Babbage (cont.)

- Proposed a more ambitious project: machine-driven Universal Calculator
- 1846 – gives up the idea of finishing difference engine no. 1 and produces drawings for Difference Engine no. 2, never built in his time
- 1847-1849 obtains gov. funds for Analytical Engine, a general purpose calculator driven by steam engine, that would be programmable, using punched cards
- Never builds a working prototype
- Project criticized by Astronomer Royal G. Airy, funds withdrawn



Swedish engineer **Georg Scheutz** (1785-1873) built his own difference engine with his son **Edvard** in 1843, following Babbage's ideas.

- He began selling them after initially predicting practically no market for computers. (e.g., one machine in 1857 bought by Dudley Obs., Albany, NY.)
- Both father and son died bankrupt

Ada Lovelace (1815-1852), daughter of poet Byron, was introduced to computing by Babbage, and in 1843 published a translation of a book with own notes on **algorithms** for the Analytical Engine.
Based on that some consider her the 1st programmer. What is certain is that she popularized the idea of applying computers outside mathematics.

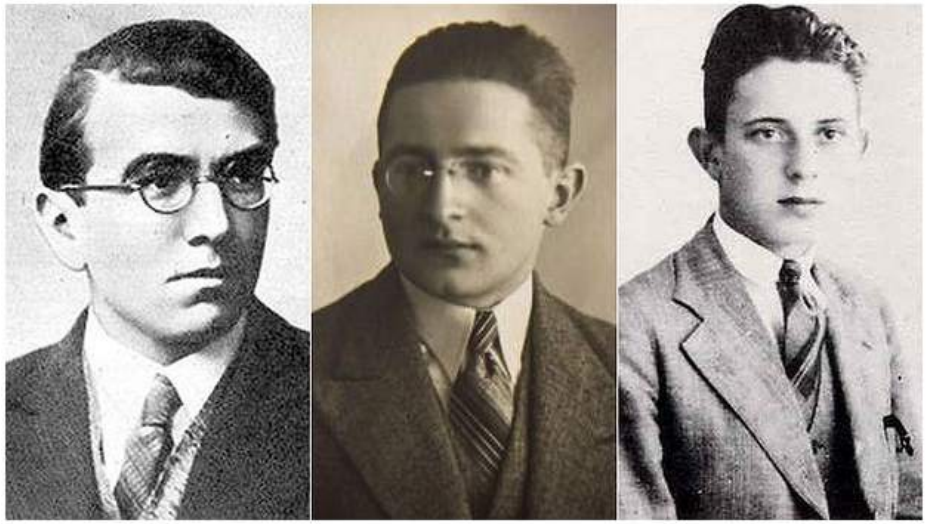
Many groups and individuals undertook the planning and construction of specialized and general, mechanical, electromechanical and electronic, programmable computers in 1930s and 1940s.

The necessity to automate the computation of possible combinations of keys coding secret cryptographic messages, to spy on an enemy, came up in the years before WWII.
https://en.wikipedia.org/wiki/Bomba_(cryptography)

- Unique breakthroughs using group-theory and a special-purpose electromechanical computer called Bomba were created by Polish Cipher Bureau mathematicians **Henryk Zygalski, Marian Rejewski,** and **Jerzy Różycki** in 1938.

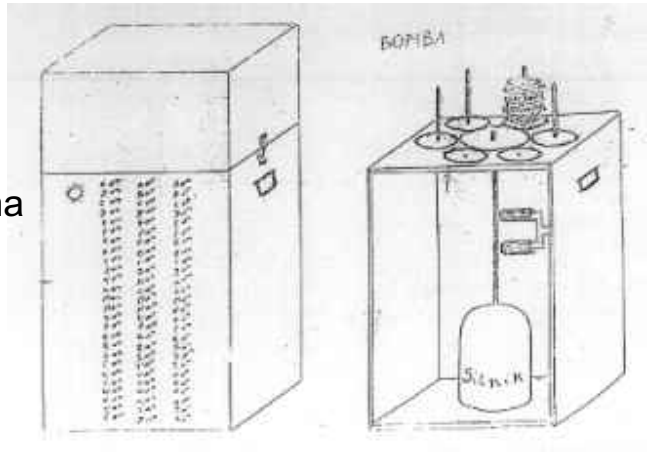
- Purpose: breaking the changing codes on ENIGMA coding machines of the German military. Their work started already in 1932 but was kept top secret even to the allied countries France and England.

Enigma
ca. 1938



Ideal location for intercepting German radio traffic was Poznań

Bomba kryptologiczna



The leader of the effort was Rejewski. Having correctly deduced the internal wiring of the Enigma machine, thanks in part to the help of French military cryptologist Gustave Bertrand, who passed manuals for ENIGMA sold to him by a German spy, Rejewski constructed the so-called cyclometer. It consisted of two Enigma copies connected together, with the position of the last coding wheel offset by three position, which allowed a streamlined brute-force search for the combinations of all 4 coding wheels (increased from 3 in the commercial version of the machine whose coding was much easier to break).

- 5 weeks before the inevitable war, Polish cryptologists presented the surprised French and British counterintelligence with copies of Enigma machines and methods to decipher the messages.

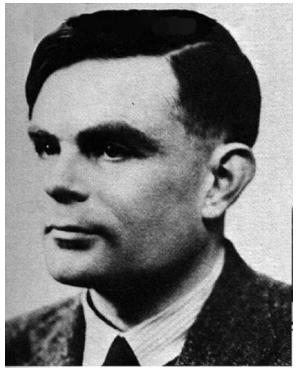
- Historians estimate that breaking of Enigma code shortened the war by 1.5 to 2.5 yrs. It probably saved hundreds of thousands of lives.

- The decryption was crucial for survival of England in early WW II

- The intense hunt for the Polish cryptologists by Gestapo (secret state police of Adolf Hitler) ensued as soon as Germany overran Poland, and later also France, to which most of the group managed to secretly move via Romania. Rejewski & Zygalski survived the hunt.

- Decryption of more complicated ENIGMA coding continued in Bletchley Park by a group led by **Alan Turing**, using more powerful electromechanical computer built there. It was also called “Bombe”. The progress was more quantitative than qualitative.

  A large number of Enigma-copies were built by Turing’s team, because the Germans occasionally upgraded their machines to introduce more complicated & secure patterns of coding, resulting in more key combinations to check.



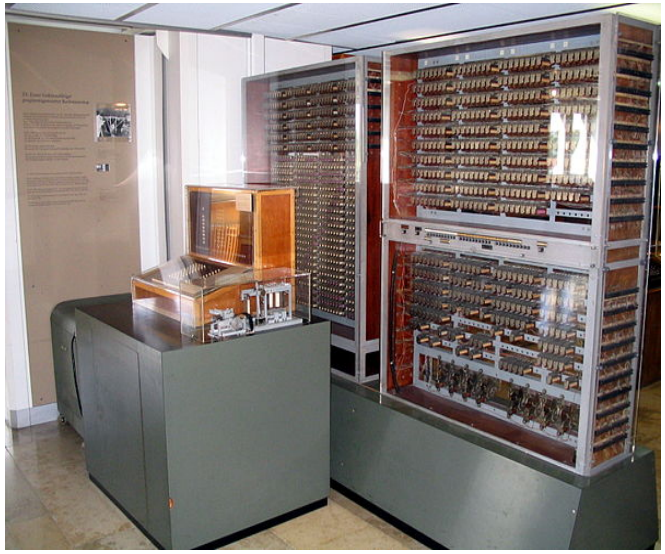
A. Turing

Bletchley Park, site of UK Government Code and Cypher School

In the flying fortress B-29 (first pressurized, high-altitude strategic bomber of WWII period, built in 1944) 5 General Electric **analog computers** allowed coordinated, remotely steered firing of defensive machine guns in electrically powered turrets. Corrections for lead and aircraft speed, altitude, humidity were taken into account, and one gunner could steer up to 3 turrets simultaneously. Analog computers were working pretty efficiently!

The first successful attempts to build a computer were sometimes classified because of war effort and national security, therefore it is difficult to clearly say “who was first”. However, the two early projects below are today considered most important.

- **Konrad Zuse** (1910-1995) single-handedly built Z3 electromechanical programmable computer in 1941
- Z3 contained 2600 relays operated on 22-bit words
- clock frequency 4-5 Hz. Code stored on punched film
- no conditional branching (no “if”)
- applied to build fully-electronic version, turned down due to war



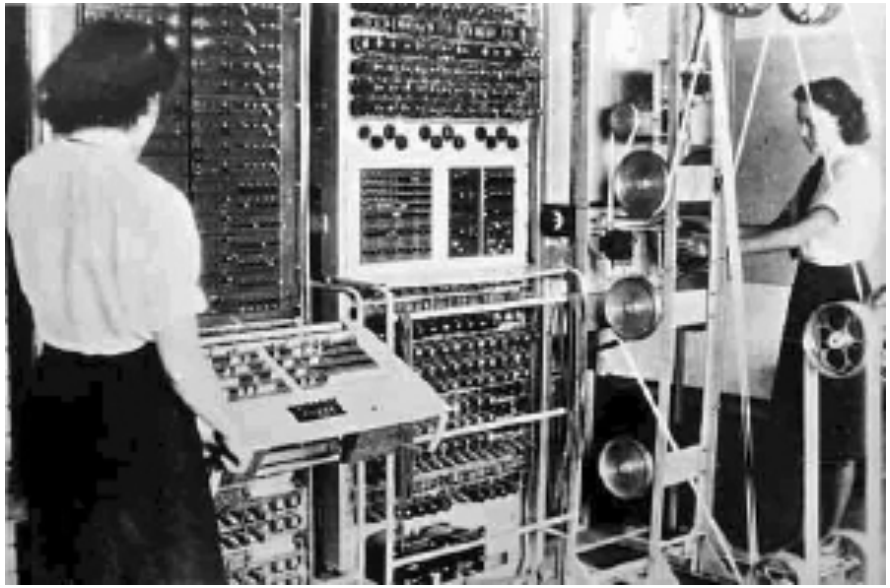
- prof. of Iowa State U. **John V. Atanasoff** and gradstudent **C. Berry**
- built in 1942 ‘ABC’ for solving systems of linear equations.
- It was non-programmable, but fully electronic
- ~300 vacuum tubes
- weight 320 kg
- used binary arithmetic, 50-bit fixed-point numbers
- had drum memory based on attached capacitors
- speed of computations ~30 FLOPS (floating point operations per second)

The 1st programmable electronic computer for decryption of messages of Lorenz SZ-40 machine called **Colossus** was built by a team of British engineers working with GC&CS (Government Code and Cypher School, Bletchley Park near London) at Post Office Research Station. Delivered in January 1944, it decoded first message on 5 Feb 1944. Colossus had 1800 vacuum tubes. The information about Colossus was classified & became partially public first in 1970s. It was designed by **Tommy Flowers.** About a hundred machines were built. To keep the new technology secret, Churchill ordered all of them destroyed after the war.

https://www.cryptomuseum.com/crypto/colossus/index.htm

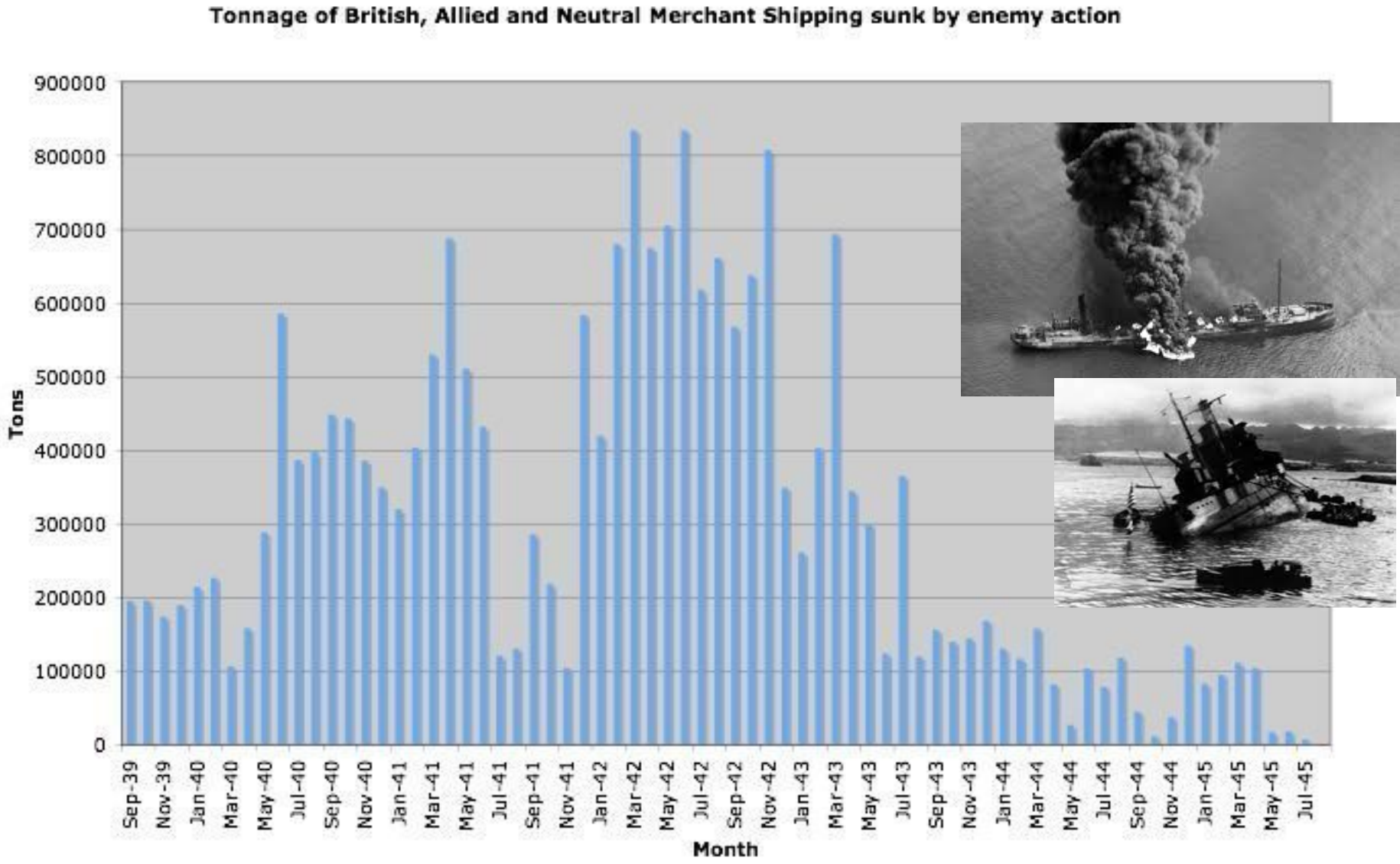
The special importance of Lorentz SZ-40 derived form it being used for telex (teleprinter) messages from High Commando of Hitler's army, i.e. for strategic information.

Early version of Colossus



Lorentz SZ-40

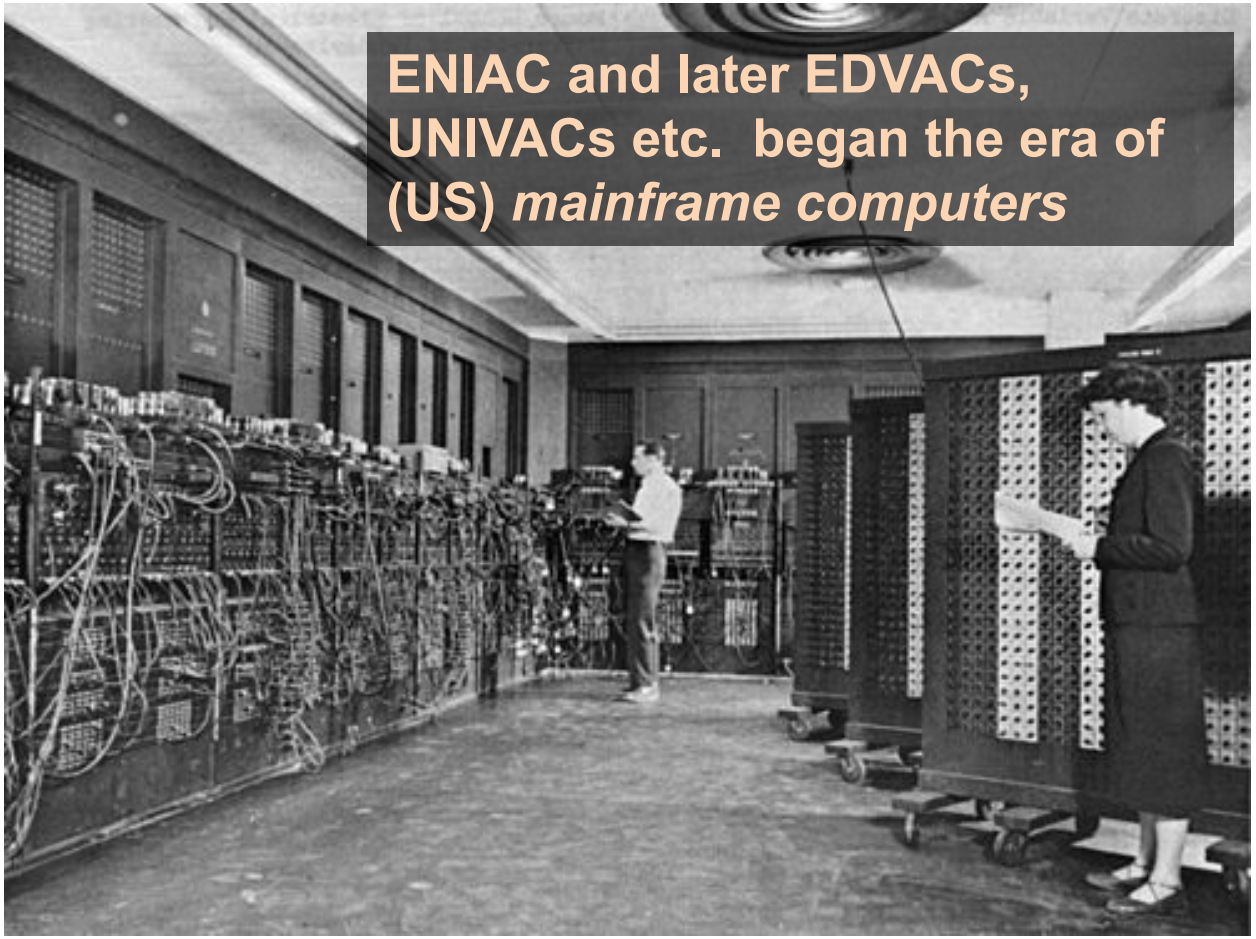
Colossus had an advanced reader + correlator of two punched paper tapes, running 32 ft/s = 5000 characters per sec. Its arithmetic speed was ~100 times larger(!)



Colossus
was built here,
rather late..

Before the information has spread about ABComputer, Z3, 'Bombe' and the Colossus of the British, it was often mistakenly stated that the first electronic computer was **ENIAC = Electronic Numerical Integrator and Computer**, built in Dec. 1946 in USA. It was used by US Army for ballistic calculations, solving differential equations of projectiles moving in air and, in secrecy, to evaluate designs of thermonuclear bombs.

Chief designers: **John Mauchley, J. Presper Eckert,** Moore School of EE, Univ. of Pennsylvania.



ENIAC was modular, had bus architecture, data buffers, and programs with conditional branching.

- 20k vacuum tubes
- 7k crystal diodes
- 10k capacitors
- 1.5k relays
- weight 30 tons
- < 300 FLOPS

It operated on decimal numbers (not binary) & consumed 150 kW power

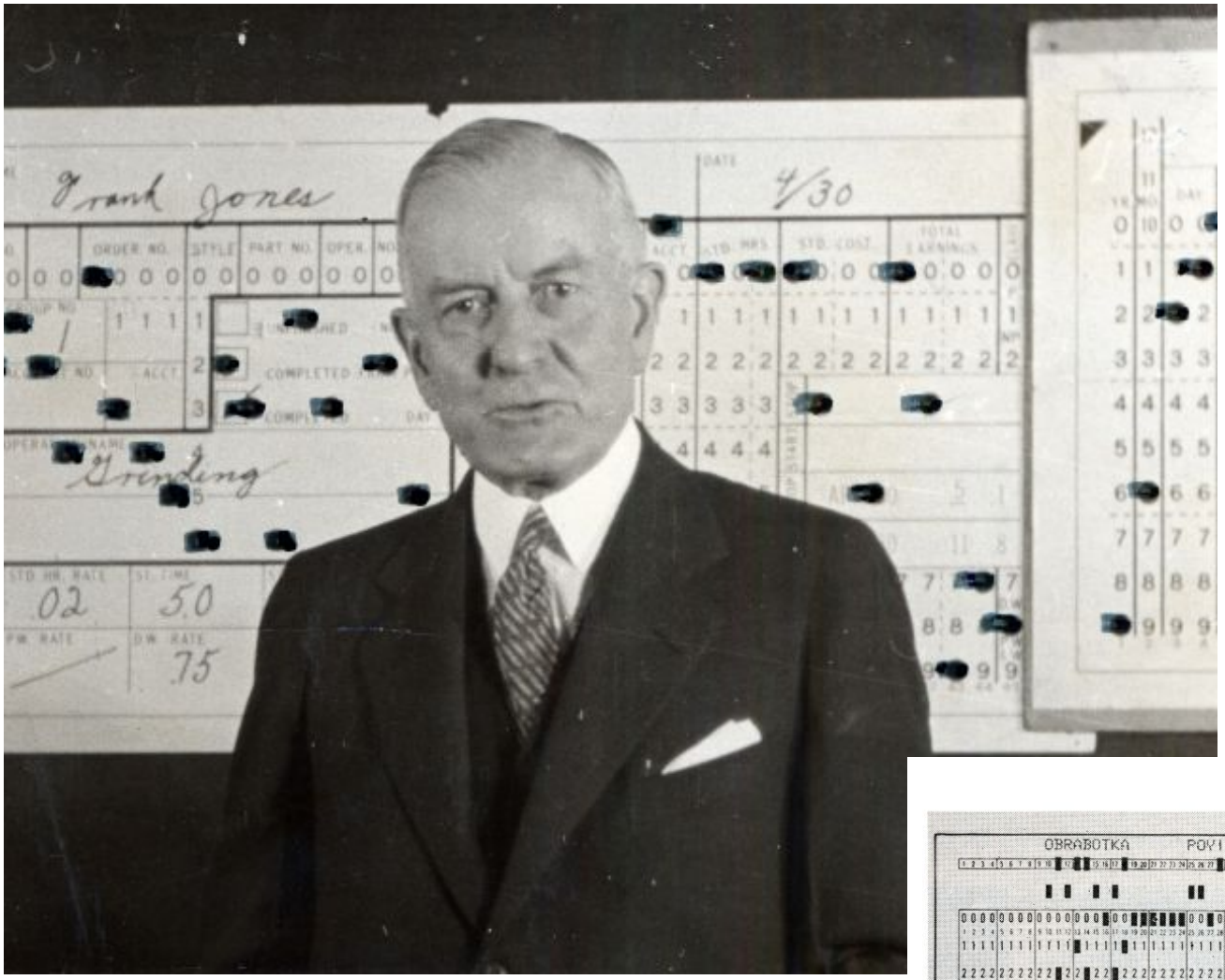
The first commercially successful mainframe (or supercomputer as we would say today) was **UNIVAC (I)**, produced by Eckert-Maulchey Computer Corporation around 1950 (later Remington Rand Co.).

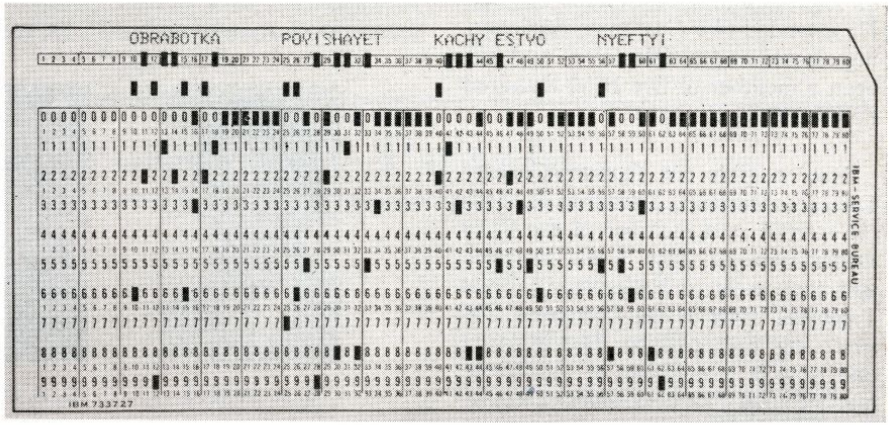
- It was used by U.S. Census Bureau in 1951
- For CBC TV station it predicted the surprising landslide win by pres. Eisenhauer in 1952 election, based on a sample of 1% voters. CBS pretended at first that Univac broke down, because the prediction sounded so impossible.
- UNIVAC had less accuracy in numeric representation than required by scientists
- It was directed toward wealthy businesses
- Migration to magnetic tape from cards was tough at first

IBM (International Business Machines Co.) up to that time produced mostly punched-card* calculators and office equipment not computers. That was to change later.

UNIVAC operator's console:

**) Hollerith (IBMs subsidiary) 80-col. cards were used by Nazis in the holocaust*





Thomas Watson (CEO of IBM in 1930s)
with the Hollerith punched cards from 1920s.

In 1928, a design with 80-columns and 10 rows (later 12) and rectangular holes, shown on the right, was adopted by IBM. It became a standard for decades.