Introduction to Scientific Computing

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Outline

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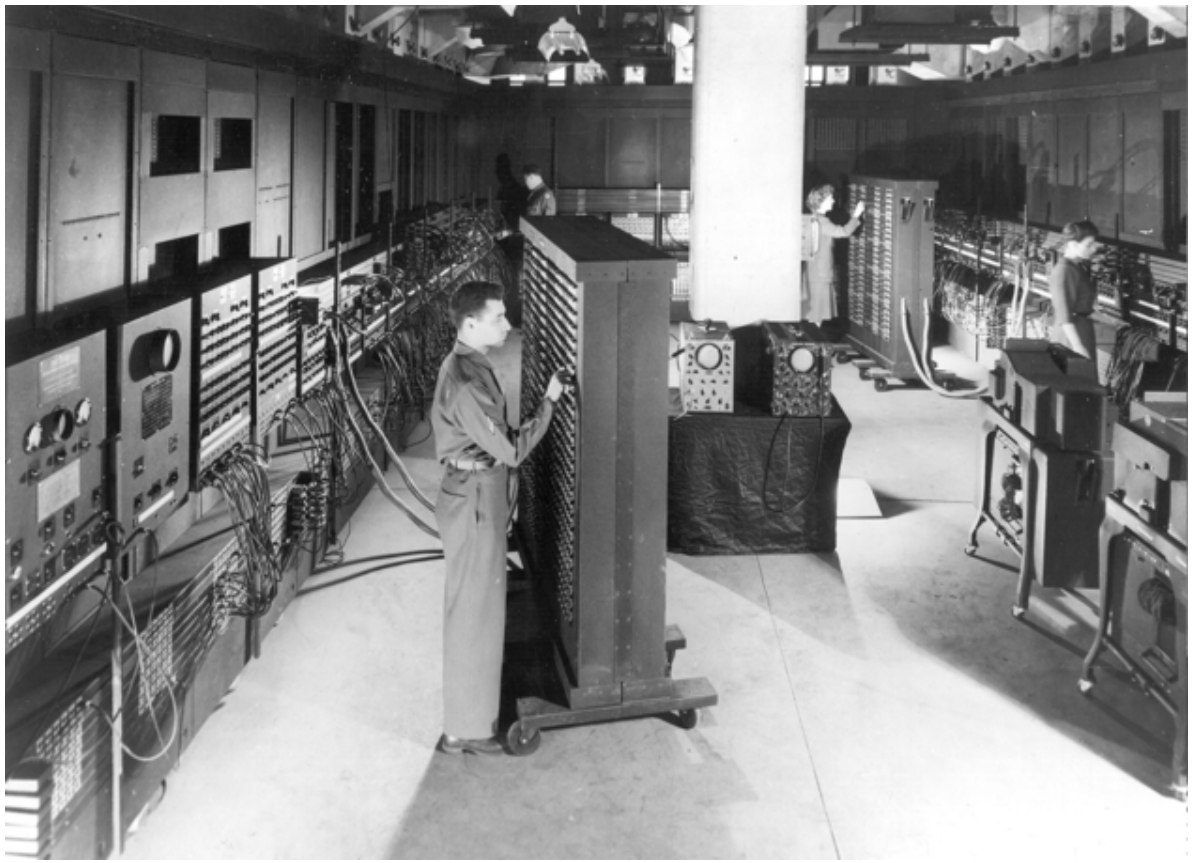
Ada Lovelace wrote the first computer program in 1842 to calculate the Bernoulli Numbers.

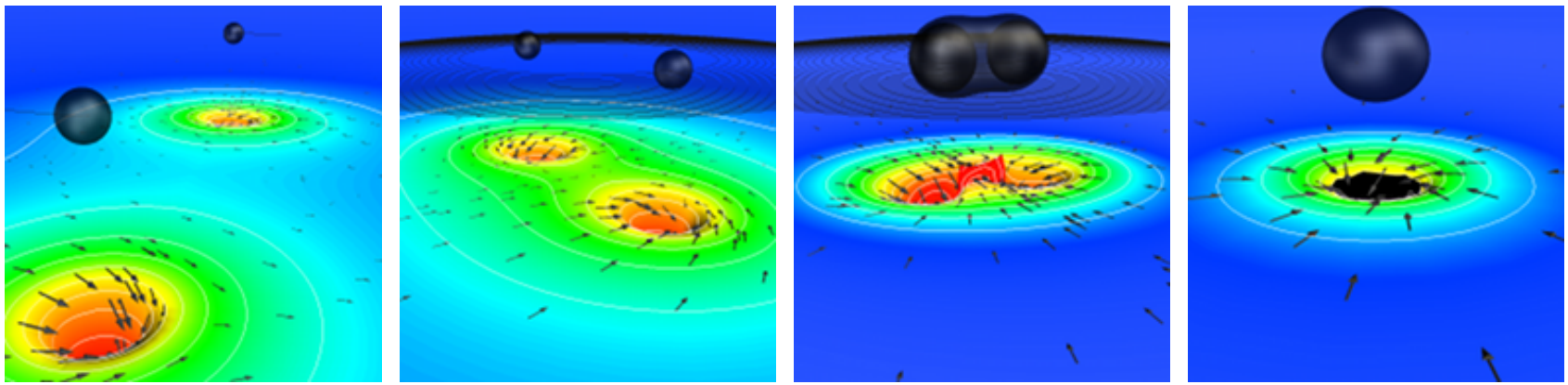
The first programmable computer was the ENIAC, used for scientific and military applications.



Margaret Hamilton led the development of the code for Apollo 11.

This code is now available on GitHub.

Today we are using supercomputers to simmulate black holes



Spectral Einstein Code (SpEC) simulation of inspiral and merger of two black holes.

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- **Differential equations** Boundary Value Problems, Initial Value Problems

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3. Write down the solution.

High-level programming provides the most straight-foward solutions

A high-level approach relies on abstraction and a programming language rich in functions.

- Python (Fuctional)
- MATLAB (Numerical)
- COMSOL (Finite Element Method)
- Mathematica (Functional)

Low-level programming provides the most efficient solutions

A low-level approach ussually requires more lines of code, but it is the way to achieve the most efficient solutions.

- Fortran (High perfomance computing, old school)
- C++ (Low-level memory management)
- Java (Multi-platform applications)

Explicit data types and memory management.

Commonly, your problem has already been solved (or at least partially solved)

The internet was invented for scientific collaboration. Google is your friend!

Here are some usefull sites

- Stack Overflow
- Stack Exchage (Super User, Mathematics, Physics)
- Physics Forums
- Online documentation

Reference books

- **Problem solving and programming Java/C++** Savitch
- **Numerical Analysis** Burden and Faires
- **Numerical Recipes** Press, Teukolsky et al
- **Spectral Methods in MATLAB** Trefethen
- **Computational Science and Engineering** Strang
- **Game Physics** Eberly

Popular Scientific Computing libraries

User firendly

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God tier

- **GSL** GNU Scientific Library for C/C++
- **Intel MKL** Math Kernel Library
- **BLAS** and **LAPACK** Linear Algebra
- **FFTW** Fastest Fourier Transform in the West
- **CUDA, OpenCL** GPU programming
- **OpenGL, Vulkan, Direct3D** graphics

Specialized Scientific Computing libraries

- **Chebfun** Numerical computing with functions
- **DistMesh** Simple mesh generator in MATLAB
- **NFFT** Non-equispaced Fast Fourier Transform
- **ARPACK** Large scale eigenvalue solver
- **SCPACK** Schwartz-Christoffel conformal mapping
- **MultiParEig** Multiparameter eigenvalue problem

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A Boundary Value Problem (BVP) is a differential equation

Find $u(x)$ that satifies a differential equation and boundary conditions. Example:

$$\frac{d^2u}{dx^2} = 1000cos(5\pi x)e^{-x^2}$$

With boundary conditions $u(-1) = 2$ and $u(1) = -1$.

Many natural-occuring BVPs are second order and linear

Linear BVP (and some non-linear) may be discretized into matrix equations.

$$Ax = b$$

Numerical linear algebra has provided many succesfull methods for scientific computing problems.