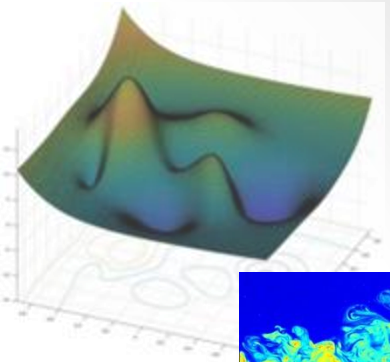
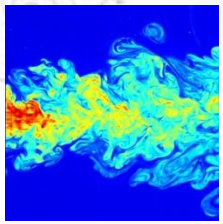
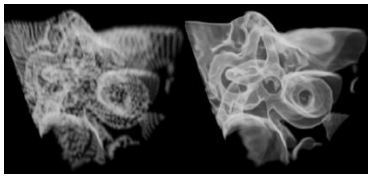
Numerical Methods







Teaching by:

- **Part I: Ljubisa Miskovic (ljubisa.miskovic@epfl.ch)**

  Tuesday, 8h15-10h,

  18.02.2025-08.04.2025

- **Part II: Kevin Sivula (kevin.sivula@epfl.ch)**

  Tuesday, 8h15-10h

  15.04.2025-27.05.2025

Exercises

Tuesdays, 10h15-11h

18.02.2025-27.05.2025

Assistants:

David Liaskos (david.liaskos@epfl.ch) **(part I)**

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Exercises

- Install Python

Evaluation, part I

Homeworks (30% of the final note):

- Several (typically three) homework
- Delivered through the Moodle: https://moodle.epfl.ch/course/view.php?id=16465

Exam (70% of the final note for Part I):

- On 16.04.2021 (tentative date)

Numerical methods

Applied math techniques aiming to solve complex mathematical problems using (mostly) basic arithmetic operations.

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Applied math techniques aiming to solve complex mathematical problems using (mostly) basic arithmetic operations.

Instead of analytical solutions, with these techniques, we obtain approximate solutions to a mathematical problem, e.g.,

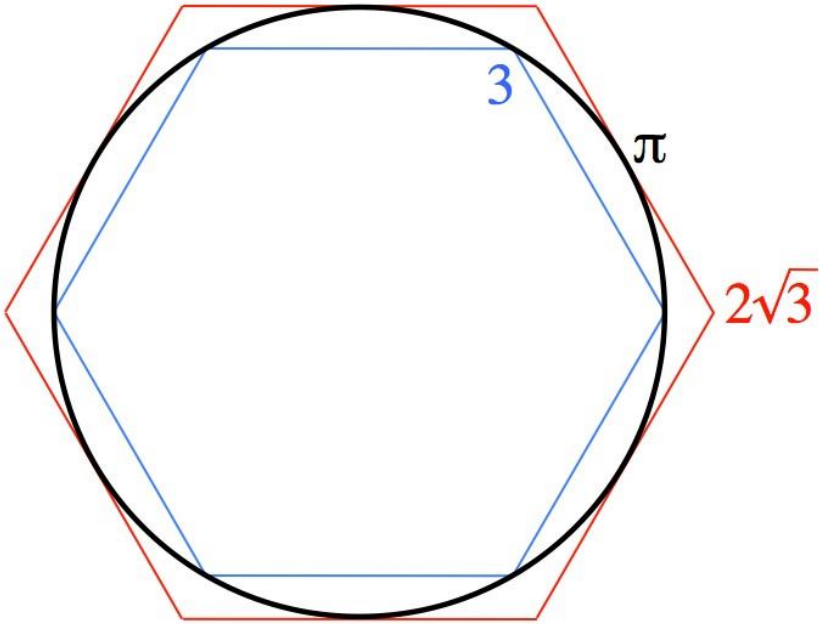
- finding roots
- solving systems of linear equations
- computing integrals
- solving ordinary differential equations (ODEs)
- …

Why do we need numerical methods?

- An analytical solution is hard or impossible to obtain or not practical (complex behavior or time costly)
- Allow you to extend the classes of problems that we can address
- Allow you to use “off-the-shelf” software to solve the problems:
  - we need to understand basic theory to use them
  - we might need to “tailor” this software to our needs

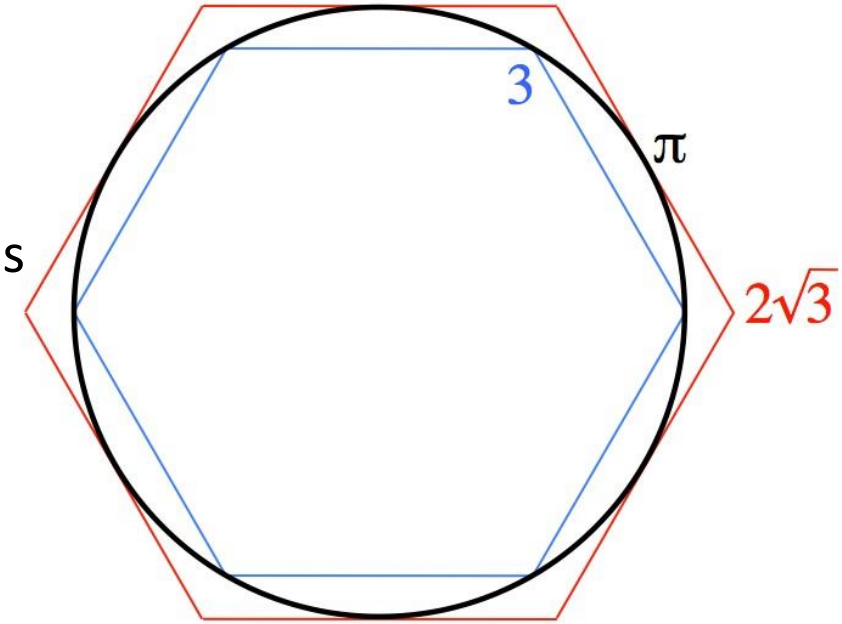
An early historical example

- In 3rd century BC, Archimedes found a way to compute π numerically



An early historical example

- In 3rd century BC, Archimedes found a way to compute π numerically
- Circle's perimeter is:
  - > than the inscribed polygon
  - < than the circumscribed polygon
- More polygon sides -> tighter bounds



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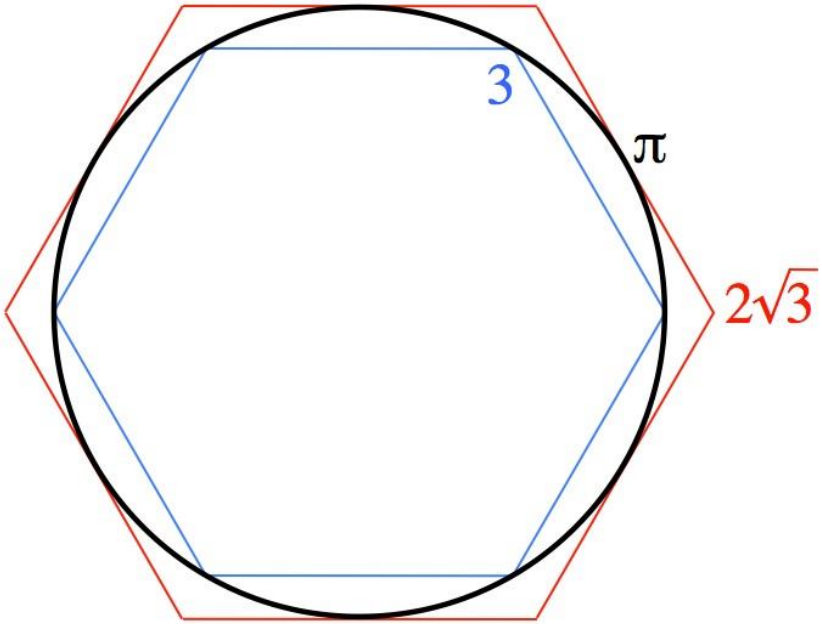
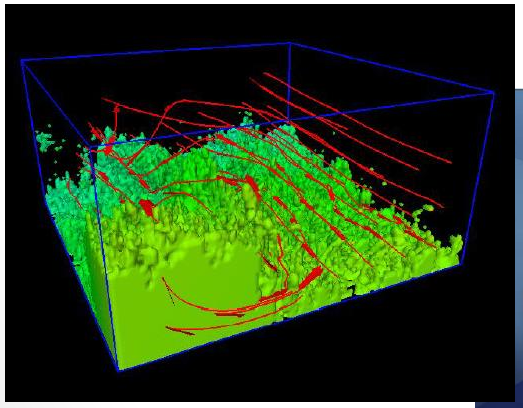
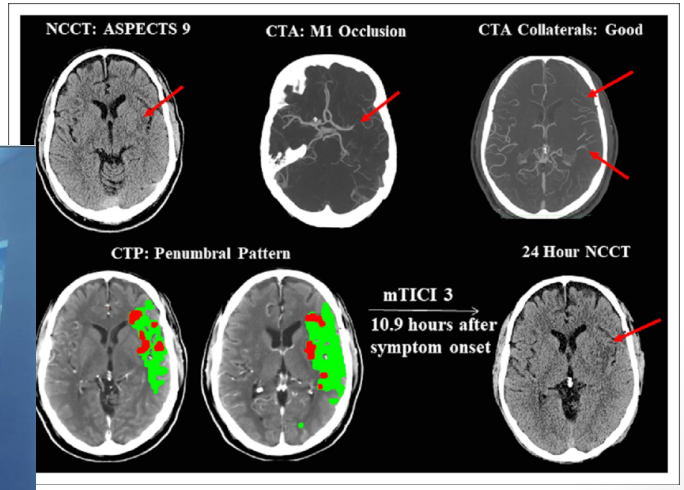


- Archimedes method:
  - $P_{2k} = \frac{2P_k p_k}{P_k + p_k}$ and $p_{2k} = \sqrt{p_k P_{2k}}$
  - starting from $p_6 = 3$ and $P_6 = 2\sqrt{3}$,
    - $k = 6$: $3 < \pi < 3.46410$
    - Iter. 1: $3.10583 < \pi < 3.21539$
    - Iter. 2: $3.13263 < \pi < 3.15966$
    - Iter. 3: $3.13935 < \pi < 3.14609$
    - Iter. 4: $3.14103 < \pi < 3.14271$
    - Iter. 5: $3.14145 < \pi < 3.14187$
    - Iter. 8: $3.141590 < \pi < 3.141597$
  - Compare to: $\pi = 3.1415926535 \ldots$

Application of numerical methods

- Some applications in general fields
  - Studying phenomena in Electromagnetics (Maxwell's equations), fluid mechanics (Navier-Stokes equations), computational biology and chemistry…
  - Computer-aided Geometic design and computer graphics (e.g., ray tracing)
  - Visualization, video and image processing





Application of numerical methods

- In chemistry and chemical engineering
  - Quantum mechanical calculations of atoms and molecules (e.g., molecular dynamics methods, Monte Carlo methods)
  - Analysis of chemical reaction kinetics
  - Acquisition and processing of Spectral Data in Molecular Spectroscopy
  - Transport processes
  - Optimization of chemical plants
  - …

How this works?

Steps in solving problems numerically:

- Formulate a mathematical model of underlying problem
- Choose a numerical method to solve the problem
- Implement in a computer environment
- Validate solutions

Numerical solutions

We have to make sure that numerical solutions are:

- Accurate:
  - Good approximate to the true value.
  - Information about the approximation error.
- Practical:
  - A solution can be found in a reasonable amount of time.

What will I learn in this course?

- **Understanding** the theoretical and practical aspects of the use of numerical methods
  - Know common numerical algorithms and their properties
    - When they can be used, their limitations and advantages
    - How they can fail
    - How they can be improved

- **Implement** numerical methods for a variety of applications

Tentative Topics (Part I)

1.	Linear equations
2.	Nonlinear equations
3.	Numerical integration
4.	Numerical differentiation
5.	Ordinary differential equations
6.	Basics of data analysis
7.	Selected exam problems