Scientific Computing

Lecture 1

Delft University of Technology

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September 4, 2024

Course Structure and Planning

▸ Course Website

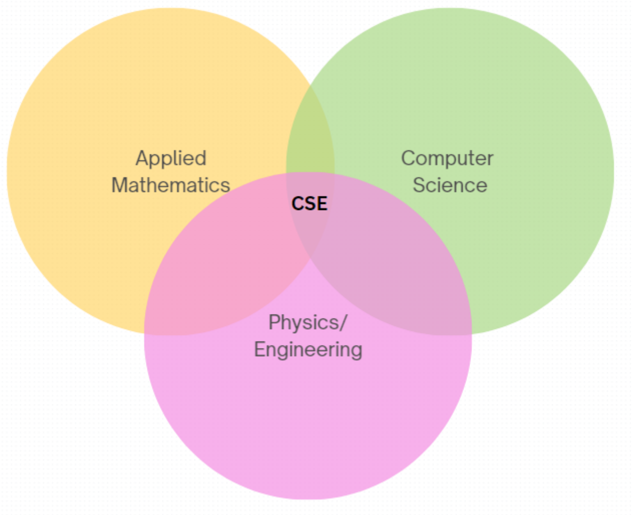
- Weekly 2-hour lecture (schedule on Brightspace)
- G_1: Take-home exam (theoretical and/or practical)
  - Deadline: 15-11-2024
- G_2: Take-home exam (mostly practical)
  - Deadline: 10-01-2025
  - Group of 2 students - PhD TA's
  - Check-in with supervisor in December
- G_3: Final written exam
  - Exam on 22-01-2025
- Final grade: $(G_1 + G_2 + 2G_3)/4$, with the condition that all grades must be ≥ 5

Prerequisite Knowledge

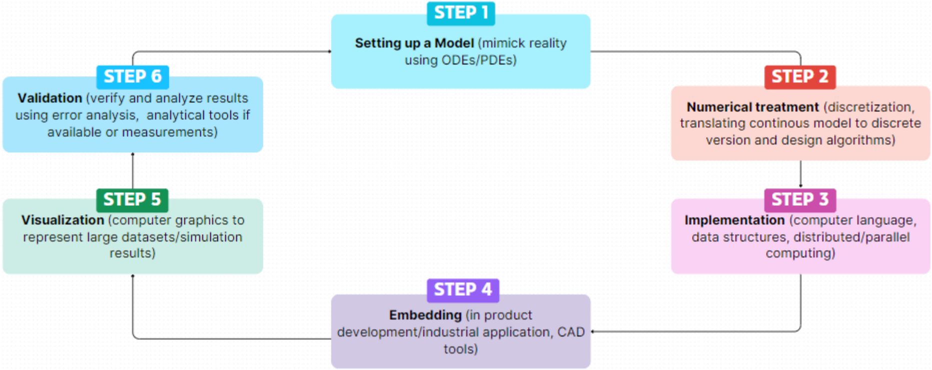
We assume you are familiar with material from the courses:

- Linear Algebra
- Calculus or Analysis
- Differential Equations
- Numerical Methods I (Book used)

Compututational Science and Engineering



Six Steps of a Simulation Process

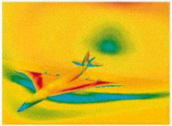


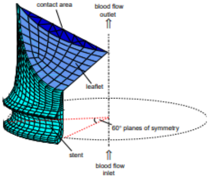
Example: Turbulence

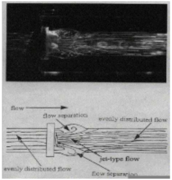
Real-world phenomena

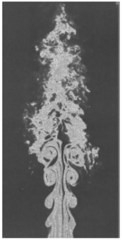
Numerical Model

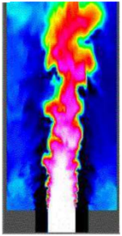
Numerical Solution











Algorithms, Methods, Code

Scientific Computing focuses on developing algorithms, defined as:

A set of instructions to carry out certain mathematical, arithmetical and logical operations (or already known algorithms) for solving a prescribed problem.

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Example: Babylonian Root Extraction

$$\sqrt{a} \ (a > 0): \quad x_0 > 0 \quad \text{arbitrary}$$
$$n = 1, 2, 3, \ldots \quad x_n = \frac{1}{2}\left(x_{n-1} + \frac{a}{x_{n-1}}\right)$$

Stopping criterion: $|x_n - x_{n-1}| \leq \epsilon$

Babylonian Root - Derivation

Desired: zeros of $g(x) = x^2 - a = 0$

Derivation via ▸ Newton-Raphson algorithm:

$$x_n = x_{n-1} - \frac{g\left(x_{n-1}\right)}{g'\left(x_{n-1}\right)}$$

$$x_n = x_{n-1} - \frac{x_{n-1}^2 - a}{2x_{n-1}} = x_{n-1} - \frac{1}{2}x_{n-1} + \frac{1}{2}\frac{a}{x_{n-1}}$$

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Infinite algorithm + stopping criterion = finite algorithm

Babylonian Root - Results

We take $a = 0.64$, $\sqrt{a} = 0.8$

n	x_n	$x_n - \sqrt{a}$	$(x_n - \sqrt{a}) / \sqrt{a}$	EB (3)
0	0.76	0.04	0.05	0.05
1	0.801052631	0.001052631	0.001316...	0.001316
2	0.800000691	0.000000691	0.000000864	0.000658
3	0.800000000...	$< 10^{-10}$	$< 1.2510^{-10}$	0.000329

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Improved Error Bound

$$\frac{x_n - \sqrt{a}}{\sqrt{a}} = \frac{1}{2}\left(\frac{x_{n-1} - \sqrt{a}}{\sqrt{a}}\right)^2 \frac{\sqrt{a}}{x_{n-1}}$$

$$\text{If } x_0 \geq \sqrt{a} : \frac{x_n - \sqrt{a}}{\sqrt{a}} \leq \frac{1}{2^{2^n - 1}}\left(\frac{x_0 - \sqrt{a}}{\sqrt{a}}\right)^{2^n}$$

Errors in Scientific Computing

'"If mathematical theories refer to reality, then they are not certain. If they are certain, then they do not refer to reality.'

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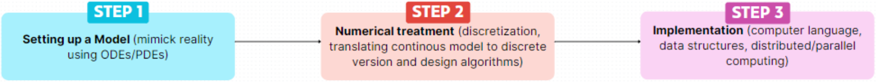
Error Measures: for $x, \hat{x} \in \mathbb{R}$:

$$|x - \hat{x}| \leq \epsilon \qquad \text{Estimate of absolute error}$$

$$\frac{|x - \hat{x}|}{|x|} \leq \epsilon \qquad \text{Estimate of relative error}$$

Sources of Errors



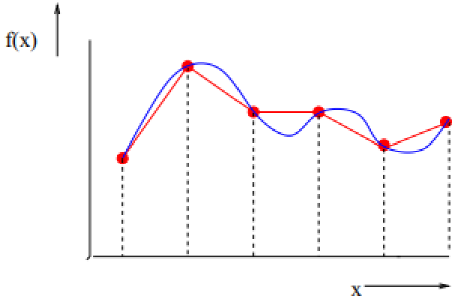
- Modelling error
- Error in data

- Discretization error
- Truncation error
- Round-off error

- Programming errors

Sources of Errors - Discretization

Discretization error



Only n values are obtained: gives an approximate solution curve.

Sources of Errors - Round-off

Numbers can only be stored with finite number of bits/digits

Generally round-off error small

Problematic when used with unstable algorithm

Sources of Errors - Round-off

Ill-conditioned linear system

$$\begin{pmatrix} 1 & 1 \\ 1 & 1-\varepsilon \end{pmatrix} x = \begin{pmatrix} 4 \\ 4-\varepsilon \end{pmatrix} \quad Ax = b$$

$$x^* = \begin{pmatrix} 3 \\ 1 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 1 \\ 1 & 1-\varepsilon \end{pmatrix} \tilde{x} = \begin{pmatrix} 4+\varepsilon \\ 4-2\varepsilon \end{pmatrix} \quad A\tilde{x} = \tilde{b}$$

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Also: $\|b-\tilde{b}\|_\infty = \varepsilon$, but $\|x-\tilde{x}\| = \max\{|2-\varepsilon|, 2\} = 2$

Sources of Errors - Round-off

Problem: Computation of

$$x_n := \int_0^1 \frac{t^n}{t+10} dt \text{ for larger } n$$
$$> 0 \text{ clearly}$$

$$x_0 = \int_0^1 \frac{1}{t+10} dt = \ln(10+t)|_0^1 = \ln\frac{11}{10} = \ln 1.1 \approx 0.0953$$

$$x_n := \int_0^1 \frac{t^n}{t+10} dt = \int_0^1 \frac{t^{n-1}(t+10) - 10t^{n-1}}{t+10} dt$$

$$= \int_0^1 t^{n-1} dt - 10x_{n-1} = \frac{1}{n} - 10x_{n-1}$$

Recursion: $x_n = \frac{1}{n} - 10x_{n-1}$

Sources of Errors - Round-off

Practically: computation with 3 decimals gives the approximations $\tilde{x}_n$

$$
\begin{aligned}
\tilde{x}_0 &= 0.0953 \\
\tilde{x}_1 &= 1 - 0.953 = 0.047 \quad (x_1 = 0.0469..) \\
\tilde{x}_2 &= 0.5 - 0.470 = 0.030 \quad (x_2 = 0.0310..) \\
\tilde{x}_3 &= 0.333 - 0.300 = 0.033 \quad (x_3 = 0.0232..) \\
\tilde{x}_4 &= 0.250 - 0.330 = -0.08 < 0! \quad (x_4 = 0.0185..)
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Reason: $x_n = \frac{1}{n} - 10x_{n-1}$, x_{n-1} contains error ε

$\Rightarrow$ x_n contains error approx. 10ε

$\Rightarrow$ x_{n+1} contains error approx. 100 . "Unstable recursion"

Sources of Errors - Round-off

Fix it: reverse procedure, start with x_n

$$x_{n-1} = \frac{1}{10n} - \frac{1}{10}x_n = \frac{1}{10}\left(\frac{1}{n} - x_n\right)$$

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How to pick x_n?

$$x_n = \int_0^1 \frac{t^n}{t+10}dt \leq \int_0^1 \frac{1}{10}t^n dt = \frac{1}{10(n+1)} \to 0 \quad (n \to \infty)$$

Employ recursion with $y_n = 0, y_{n-1} = \frac{1}{10}\left(\frac{1}{n} - y_n\right)$

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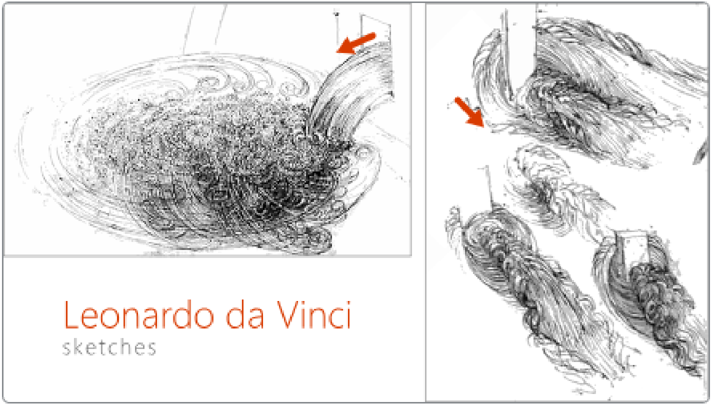
$$
\begin{aligned}
y_8 &= 0 \\
\tilde{y}_7 &= 0.0125 \\
\tilde{y}_6 &= 0.0143 - 0.00125 = 0.0131 \\
\tilde{y}_5 &= 0.0167 - 0.00131 = 0.0154 \\
\tilde{y}_4 &= 0.0200 - 0.00154 = 0.0185
\end{aligned}
$$

$\tilde{y}_4$ is 3 digits accurate

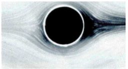
Example: Turbulence

Fluid mechanics: laminar (Euler equations) - turbulent flow (Navier-Stokes equation)

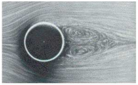


Example: Turbulence

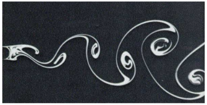
Reynolds Number represents balance between friction and non-friction



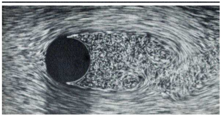
$Re = 0.16$,
Laminar, stationary, symmetric



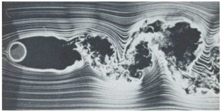
$Re = 26$,
Laminar, stationary, recirculation



$Re = 140$,
Transition, unsteady, von Kármán vortex street



$Re = 2000$,
Turbulent, unsteady



$Re = 10000$,
Turbulent, unsteady

Example: Turbulence - Mathematical Model

Flow mathematically modelled by the Navier-Stokes equation:

$$\underbrace{\frac{\partial u}{\partial t}}_{acceleration} + \underbrace{u\frac{\partial u}{\partial x}}_{convection} + \underbrace{v\frac{\partial u}{\partial y} + w\frac{\partial u}{\partial z}} + \underbrace{\frac{\partial p}{\partial x}}_{pressuregradient} =$$

$$\underbrace{\frac{1}{Re}\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}\right)}_{friction}$$

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Incompressible flow, also continuity equation:

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- $Re = \bar{U}L/\nu$ is the Reynolds number
- System of non-linear PDEs. **No** analytical solution exists (only for simple geometries/BCs).
- Solve using DNS (Direct Numerical Simulation)

Example: Turbulence - Reynolds Number

$Re = \bar{U}L/\nu$ is the Reynolds number

- Spoon stirring in a cup coffee ($Re \sim 10^4$)
- Airflow around a car ($Re \sim 3 \times 10^6$)
- Water flow in a river ($Re \sim 10^7$)
- Air flow around an aircraft ($Re \sim 3 \times 10^8$)

Example: Turbulence - DNS

How many computing operations to simulate a channel flow with $Re = 10^5$?

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How many computing operations to simulate a channel flow with $Re = 10^5$?

- Have number of grid points in all 'Eddies'
- Smallest length-scale: $\eta \approx L/1000$, i.e. 1000 gridpoints in every coordinate direction.
- In 3D this gives 10^9 number of unknowns (nou).

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Computer storage $> 10\times$ nou $= 10^{10}$

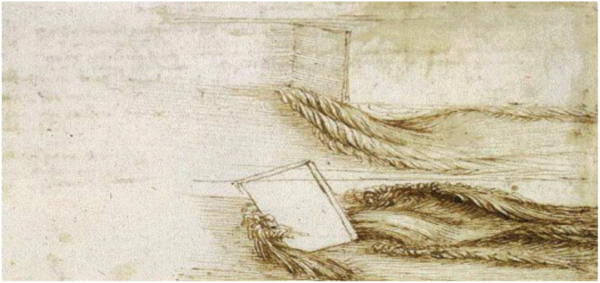
Computing operations $\sim 500\times$ nou per timestep $= 5 \times 10^{11}$

Number of timesteps $\sim 10^4$

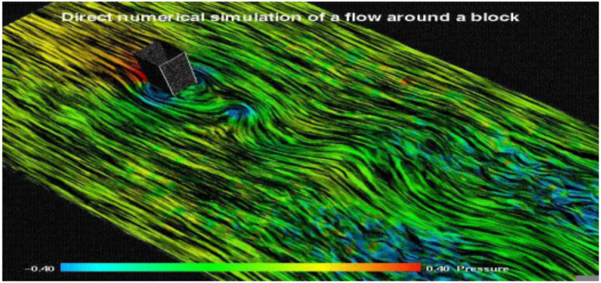
Total number of operations: 5×10^{15}

Example: Turbulence

Leonardo vs. DNS ($Re = 22000$)



Leonardo



DNS