

# POLITECNICO MILANO 1863

DEPARTMENT
OF CHEMISTRY MATERIALS
AND CHEMICAL
ENGINEERING

## Calcoli di Processo dell' Ingegneria Chimica

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#### Resources

#### Books:

- ► G., Buzzi Ferraris; Manenti, Flavio. Fundamentals and Linear Algebra for the Chemical Engineer: Solving Numerical Problems.
- ► G., Buzzi Ferraris; Manenti, Flavio. Interpolation and Regression Models for the Chemical Engineer: Solving Numerical Problems.
- ► G., Buzzi Ferraris; Manenti, Flavio. Nonlinear Systems and Optimization for the Chemical Engineer: Solving Numerical Problems.
- ► G., Buzzi Ferraris; Manenti, Flavio. Differential and Differential-Algebraic Systems for the Chemical Engineer: Solving Numerical Problems.

▶ J. Nathan Kutz. Data-Driven Modeling and Scientific Computation.

- Steven L. Brunton; J. Nathan Kutz. Data-Driven Science and Engineering: Machine Learning, Dynamical Systems, and Control.
- ▶ A. Quarteroni; R. Sacco; F. Saleri; P. Gervasio. Matematica Numerica.
- ► A. Quarteroni; F. Saleri; P. Gervasio. Calcolo Scientifico: Esercizi e problemi risolti con MATLAB e Octave.
- ▶ D. Manca. Calcolo numerico applicato.

#### Online Material:

- ▶ Numerical Methods applied to chemical engineering (MIT).
- ► GitHub repository of the practical sessions.
- ► Matlab online tutorial and documentation.

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Remember, every time we use smart devices, some code is running in the background. Moving a mouse pointer from one part of your computer screen to the other may seem like a simple task, but in reality, so many lines of code just ran. An act as simple as typing letters into Google Docs leads to lines of code being executed in the background. It's all code everywhere.

## The Natural Language of Computers

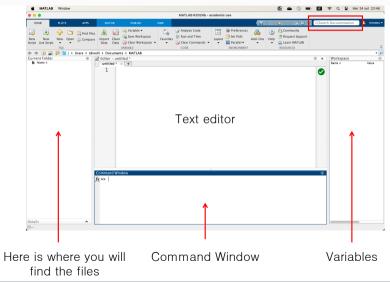


Figure 1: Cleve Barry Moler

The <u>only</u> language understood by a computer is the machine language. A very long list of 0 and 1. However it is a little bit inconvenient to write a series of zeros and ones. So (very smart) people, like the one in the picture, invented what are called programming languages (C/C++, Fortran, python, julia, MATLAB, ...).

N.B. Computers aren't very smart, the instructions need to be very precise! Telling a computer what you want it to do is sometimes hard because you have to explain things very carefully and precisely.

#### **MATLAB**



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▶ By default, MATLAB store all values as double-precision floating point.

### Area of a cylinder

Let's compute the area of a cylinder given the diameter D = 20 cm and height h = 50 cm.

### Code:

## What happens:

- 1. Create variable **D** = 0.2 m
- 2. Create variable h = 0.5 m
- 3. Calculate **perimeter** =  $\pi \times 0.2$
- 4. Calculate Area = perimeter  $\times$  0.5

### Source code: scripts and functions in MATLAB

Scripts are m-files (text format) containing MATLAB statements. MATLAB "functions" are another type of m-file. The biggest difference between scripts and functions is that functions have input and output parameters. Script files can only operate on the variables that are "hard-coded" into their m-file.

```
1 D = 0.2;  % m
2 h = 0.5;  % m
3 perimeter = pi * D;
4 Area = perimeter * h;

ans = 0.3142

function Area = ComputeArea(D, h)
perimeter = pi * D;
Area = perimeter * h;
end

ComputeArea(0.2, 0.5)
```

Introduction to Matlab 11

ans = 0.3142

#### Variables names

- ► MATLAB is case sensitive! Pippo  $\neq$  pippo
- ➤ Variables name should be self explanatory, so prefer distance, radius, ... than a, b, ...
- ▶ When possible <u>use</u> the camel case notation to make stuff easier to read. PipeLength, GasTemperature, ....

### **Arrays and Matrices**

► In MATLAB arrays are defined as:

▶ Matrices can be defined as a set of stacked arrays separated with ;

```
M = [5 13 97; 31 98 36; 11 9 20]
```

```
M = 5 13 97 31 98 36 11 9 20
```

▶ Elements can be accessed using their index (indices in MATLAB starts from 1)

v(1)

ans = 5

M(2,1) % (row number, column number)

ans = 31

# Creating arrays and matrices

► Create a matrix of zeros or ones:

$$A = ones(2,3)$$

1
1

► Create a vector of **n** equally spaced elements:

```
v1 = [1:2:11] % Parenthesis can be omitted
v1 = 1 \quad 3 \quad 5 \quad 7 \quad 9
                                       11
v2 = [1:3:11] % Parenthesis can be omitted
v^2 = 1 	 4 	 7 	 10 	 % be careful!
v3 = linspace(1,10,6) % Parenthesis can NOT be omitted!
v3 = 1.0 2.8 4.6 6.4 8.2
                                                 10.0
```

# Operations with arrays and matrices

► Size of a matrix:

$$M = [1 \ 2 \ 3; \ 4 \ 5 \ 6]$$
  
size(M)

ans = 
$$2 3$$

► Copying a matrix:

$$A = M$$

6

► Copying a line or a column of a matrix:

$$V = M(1,:)$$

► Size of an array:

ans = 
$$1 3$$

$$ans = 3$$

► Matrix transposition:

$$C = B'$$

1 4 2 5 3 6

► Element wise multiplication:

► Matrix multiplication:

Error using \* Inner matrices dimensions must agree.

N.B. 
$$size(M) = 2 3$$
;  $size(C) = 3 2$ 

Thank you for the attention!