POLITECNICO
MILANO 1863

DEPARTMENT
OF CHEMISTRY MATERIALS
AND CHEMICAL
ENGINEERING

Introduction to MATLAB

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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What is programming?

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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

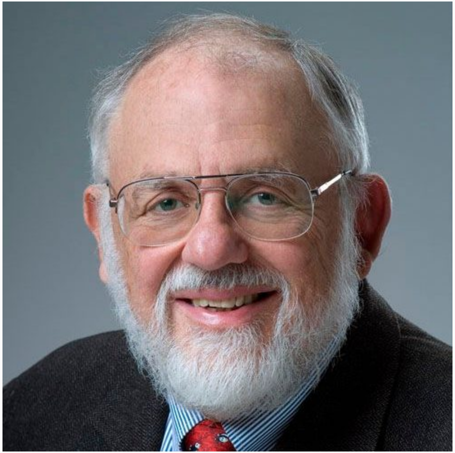
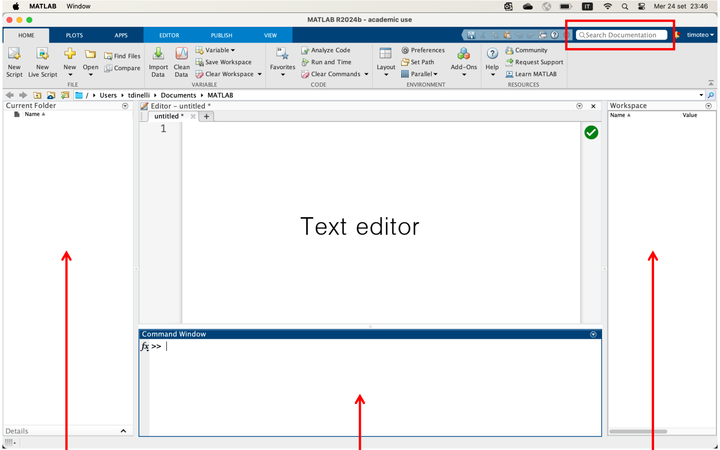


Figure 1: Cleve Barry Moler

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



Here is where you will find the files

Command Window

Variables

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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:

```
D = 0.2;          % m (diameter)
h = 0.5;          % m (height)
perimeter = pi * D;
Area = perimeter * h;
```

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.

```
D = 0.2;          % m
h = 0.5;          % m
perimeter = pi * D;
Area = perimeter * h;
```

```
ans = 0.3142
```

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

```
ComputeArea(0.2, 0.5)
```

```
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 use the camel case notation to make stuff easier to read. PipeLength, GasTemperature, ...

Arrays and Matrices

- In MATLAB **arrays** are defined as:

```
v = [5 13 97 31 98]
```

```
v =

     5    13    97    31    98
```

- **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 = zeros(3,2)
```

```
A =

     0     0
     0     0
     0     0
```

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

```
A =

     1     1     1
     1     1     1
```

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

```
v1 = [1:2:11]  % Parenthesis can be omitted
```

```
v1 =      1      3      5      7      9      11
```

```
v2 = [1:3:11]  % Parenthesis can be omitted
```

```
v2 =      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
```

```
A =
        1       2       3
        4       5       6
```

- Copying a line or a column of a matrix:

```
v = M(1,:)
```

```
v =
        1       2       3
```

- Size of an array:

```
size(v)
```

```
ans = 1 3
```

```
length(v)
```

```
ans = 3
```

- Matrix transposition:

```
C = B'
```

```
C =
        1       4
        2       5
        3       6
```

- Element wise multiplication:

```
M .* M
```

```
ans =
        1       4       9
        16      25      36
```

- Matrix multiplication:

```
M * B
```

Error using * Inner matrices dimensions must agree.

```
M * C
```

```
ans =
14      32
32      77
```

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

Loops and conditional statements

for loop

- The **for** loop repeats a series of instructions a fixed number of times.

```matlab
for i = 1:10
    paperino(i) = i;
end
```

```
paperino = 1
paperino = 1 2
paperino = 1 2 3
...
paperino = 1 2 3 4 5 6 7 8 9
paperino = 1 2 3 4 5 6 7 8 9 10
```

- The index of the **for** loop can be changed by an arbitrary increment:

```
for i = 10:-1:1
    pluto(i) = i;
end
```

```
pluto = 0 0 0 0 0 0 0 0 0 10
pluto = 0 0 0 0 0 0 0 0 9 10
pluto = 0 0 0 0 0 0 0 8 9 10
...
pluto = 0 2 3 4 5 6 7 8 9 10
pluto = 1 2 3 4 5 6 7 8 9 10
```

Examples

- Sum the first hundred natural numbers.

$$\sum_{i=1}^{100} i = ?.$$

- Sum hundred times one.

$$\sum_{i=1}^{100} 1 = ?$$

```
sum = 0;
for i = 1:100
    sum = sum + i;
end
disp(sum);
```

```
sum = 0;
for i = 1:100
    sum = sum + 1;
end
disp(sum);
```

while loop

- The **while** loop repeats a series of instructions until a condition is TRUE.
- N.B. pay attention with the while loop it can run till infinite, handle with care.

```
result = 0;
token = 0;
while (sum < 325)
    token = token + 1;
    result = result + token;
end
disp(['Iteration number: ', num2str(token)]);
disp(['Sum is equal to:  ', num2str(result)]);
```

```
Iteration number: 25
Sum is equal to: 325
```

IF Statement

- The IF statement executes a series of instructions only IF a condition is TRUE:

```
if (condition)
    % instructions
elseif (condition)
    % instructions
elseif (condition)
    % instructions
else
    % instructions
end
```

Example: Write a simple script to compute the absolute value of a number.

```
x = 35;
if (x >= 0)
    abs = x;
else
    abs = -x;
end
```

Functions

In MATLAB, a function is a block of code that takes inputs, performs a set of operations, and returns outputs. Functions allow you to organize code in a clearer and more reusable way, especially when you need to perform the same operation in different parts of your program.

Why using functions?

- **Modularity**: Separating code into functions makes the program more readable and easier to maintain.
- **Reusability**: A function can be reused in different parts of the program without rewriting the code.

Syntax

```
function [y1, ..., yN] = function_name(x1, ..., xM)
% ...
% ...
% ...
% Some code
% ...
% ...
% ...
end
```

Input variables.

Name of the function (user defined).

Output variables (parenthesis can be omitted).

The Babylonian method

Let's write a script implementing the Babylonian method to compute the square root of a number with a precision of four decimal figures, then wrap this code into a function.

1. **Make an Initial guess**. Guess any positive number x_0.
2. **Improve the first guess**. Apply the formula $x_1 = \frac{x_0 + \frac{S}{x_0}}{2}$. The number x_1 is a better approximation to $\sqrt{S}$.
3. **Iterate until convergence**. Apply the formula $x_{n+1} = \frac{x_n + \frac{S}{x_n}}{2}$ until the convergence is reached.

Convergence is reached when the digits of x_{n+1} and x_n agree to as many decimal places as you desire.

Implementation

```
function SquareRoot = ComputeSquareRoot(S)
    iter = 0;
    x0 = S;
    y = 0.5 * (x0 + S/x0);

    while abs(x0-y) > 1e-4 && iter < 50
        x0 = y;
        y = 0.5 * (x0 + S/x0);
        iter = iter + 1;
    end

    disp(['Number of iteration to reach convergence: ', num2str(iter)])
    SquareRoot = y;
end
```

Thank you for the attention!