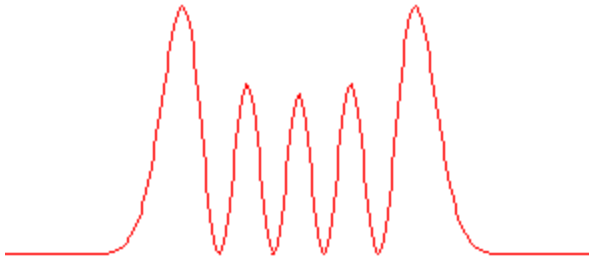
EP547 Computational Methods in QM

Topic 0

The Course



Department of
Engineering Physics

University of Gaziantep

Feb 2013

Content

- **Introduction**
- **The Course**
- **Computer Programming**
- **MATLAB Installation**
- **A Very Basic MATLAB Tutorial**

Introduction

- ***Computer programming*** **and numerical methods are an essential part of the work of many scientists and engineers.**

- **The course attempts to place emphasis on numerical methods in Non-Relativistic and Relativistic Quantum Mechnaics.**

- **We will learn MATLAB Programming Language at basic level**
  - ***MATLAB is a high-level computer language for scientific computing and data visualization built around an interactive programming environment.***

The Course

- **Course web page**
  http://www.gantep.edu.tr/~bingul/ep547

- **Also search *Google* and *Wikipedia* for any of the expressions used in this course.**

Course Content

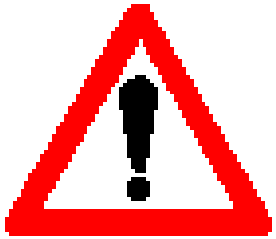
- Basic MATLAB Tutorial

- Solutions of Linear Algebraic Equations
- Symbolic and Numerical Differentiation / Integration
- Roots of Equations & Optimisation
- Numerical Methods for Ordinary Differential Equations
- Boundary Value & Eigen Value Problems
- Fourier Transform
- Monte Carlo Methods

- Overwiev of QM
- Numerical Solutions of Schrödinger Equation
- Example Applications

Computer Labs

- We'll use MATLAB under Windows operating system
- Every week you should write a few programs yourself in the lab (and more in your free time).
- So you may need to save them on a flash drive or on the internet.



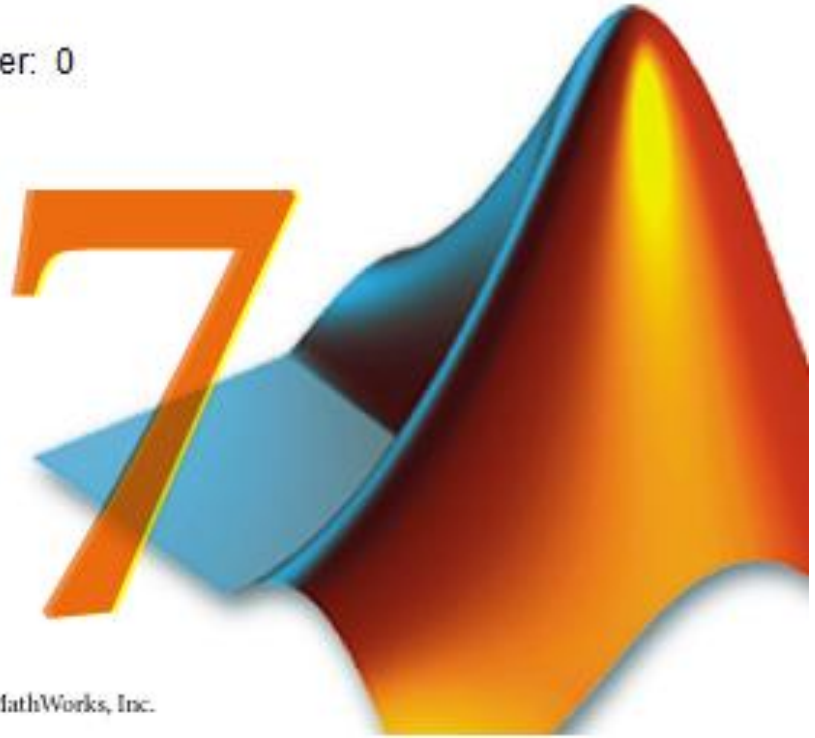
DO NOT FORGET TO BRING
YOUR LAPTOP or FLASH DISK WITH YOU

MATLAB®

The Language of Technical Computing

Version 7.0.0.19920 (R14)
May 06, 2004

License Number: 0
Ahmet
GU



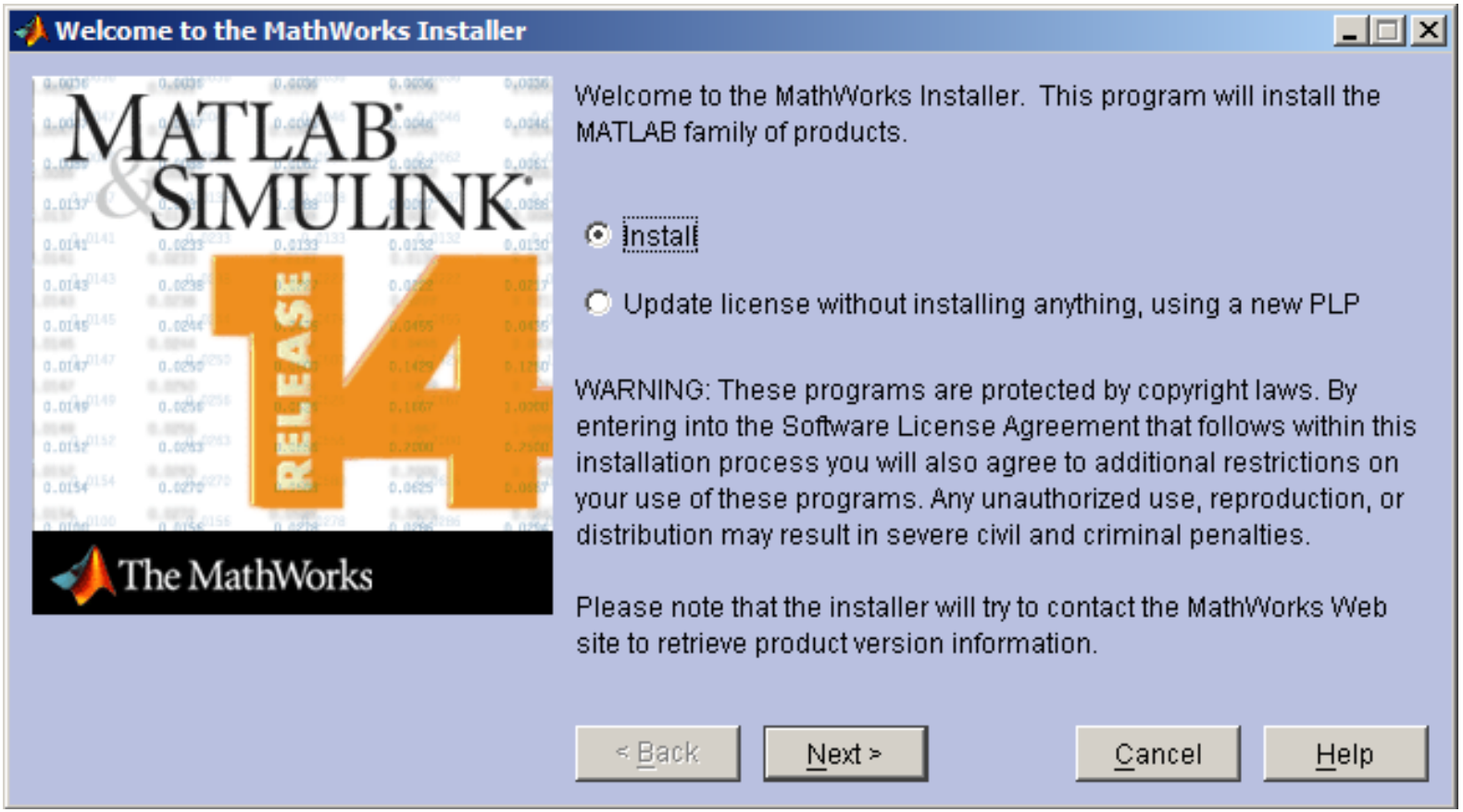
What is MATLAB?

See **http://en.wikipedia.org/wiki/MATLAB**

- MATLAB is a high-performance language for technical computing.
- It integrates computation, visualization, and programming in an easy-to-use environment where problems and solutions are expressed in familiar mathematical notation.

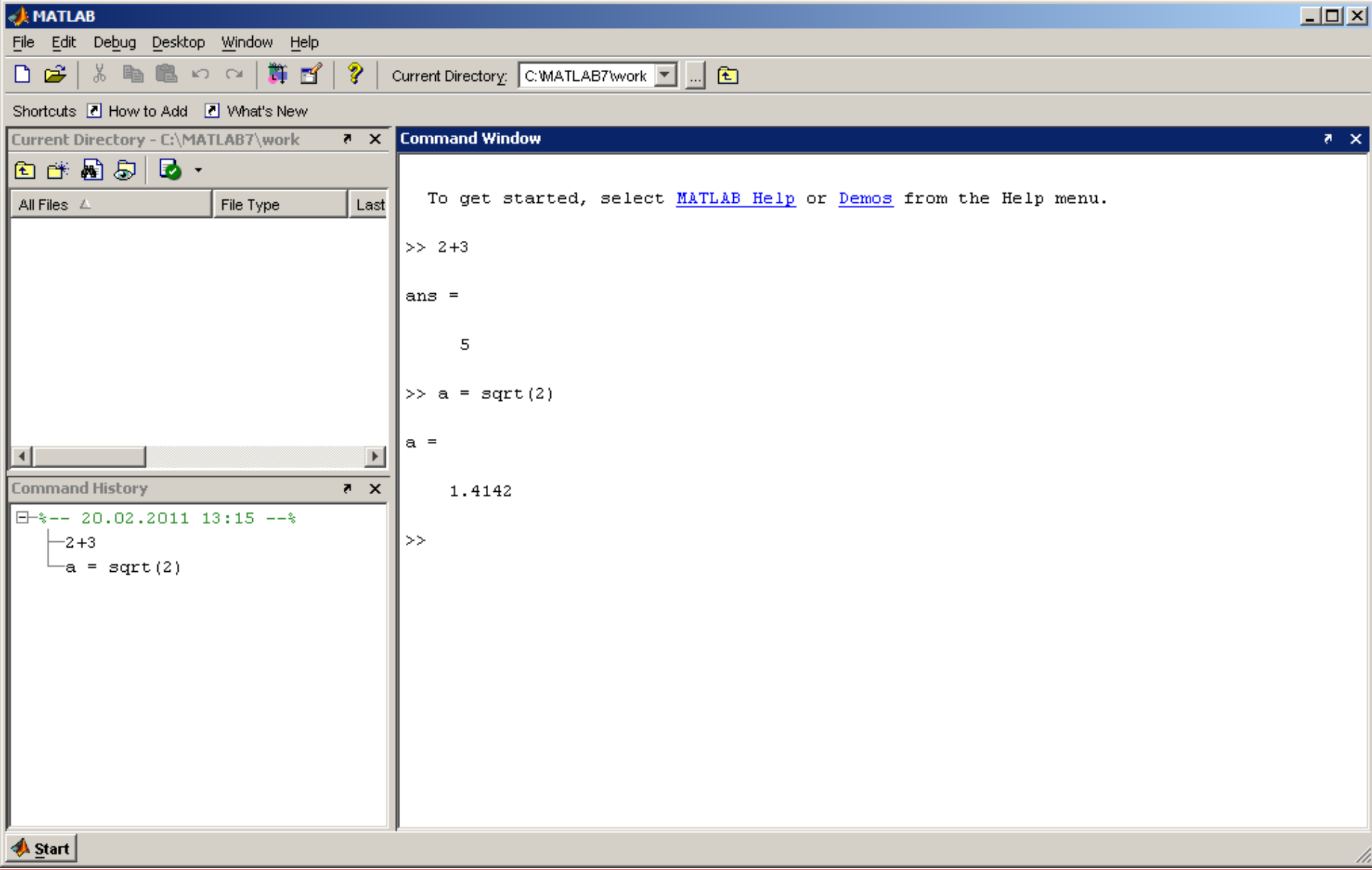
- Typical uses include
  - Math and computation
  - Algorithm development
  - Data acquisition Modeling,
  - simulation, and prototyping
  - Data analysis,
  - Scientific and engineering graphics
  - …

MATLAB 7 Installation



Follow the instructions ...

MATLAB 7 Run


MATLAB
File Edit Debug Desktop Window Help
Current Directory: C:\MATLAB7\work
Shortcuts How to Add What's New
Current Directory - C:\MATLAB7\work
All Files File Type Last
Command History
%-- 20.02.2011 13:15 --%
2+3
a = sqrt(2)
Command Window
To get started, select MATLAB Help or Demos from the Help menu.
>> 2+3
ans =
5
>> a = sqrt(2)
a =
1.4142
>>
Start

A Very Basic MATLAB Tutorial

Arithmetic works as expected.

Note that the result is given the name "ans" each time

```
>> 2 + 3
ans = 5
```

```
>> 1234/5786
ans = 0.2133
```

```
>> 2^5
ans = 32
```

You can choose your own names

```
>> a = sqrt(2)
a = 1.4142
```

```
>> x = 2 + 3i
x = 2.0000 + 3.0000i
```

```
>> y = sin(pi/2)
y = 1
```

```
>> A = [5 -3 4 2]
A = 5    -3     4     2
```

```
>> A = [5, -3, 4, 2]
A = 5    -3     4     2
```

A semicolon (;) suppresses printout of intermediate results

```
>> y = sin(pi/2);
>>
```

```
>> A = [5 -3 4 2];
>>
```

```
>> dizi = 1:7
dizi = 1      2      3      4      5      6      7
```

```
>> dizi2 = -5:2:5
dizi2 = -5    -3      -1      1      3      5
```

```
>> M = [9 8 7;  6 5 4;  3 2 1]
M =
     9      8      7
     6      5      4
     3      2      1
```

```
>> solve('2*x*x-10=0')
ans =
     5^(1/2)
    -5^(1/2)
```

```
>> int('sin(x)','x')
ans =
      -cos(x)
```

```
>> int('sin(x)','x',0,pi)
ans =
      2
```

Using M-Files

Programs can be created with the MATLAB or Notepad editor and saved with the .m extension (M-files).

Here is an example m-file (saved on desktop as ciz.m):

```
x = -10:0.1:10;
plot(x,sin(x))
hold on;
z = cos(x);
plot(x,z,'k')
```

```
>> ciz
>>
```

References

[1]. http://www.mathworks.com/products/matlab

[2]. Numerical Methods in Engineering with MATLAB,
J. Kiusalaas, Cambridge University Press (2005)

[3]. Numerical Methods for Engineers, 6th Ed.
S.C. Chapra, Mc Graw Hill (2010)