CHE656 Course Slides

(10th Edition, 2020)

Modeling in Chemical Engineering with MATLAB

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Introduction

What Is MATLAB?

- MATLAB = Matrix Laboratory
  - by The MathWorks, Inc. (www.mathworks.com)
- Originally developed for easy matrix manipulation
- Latest: Version R2020a (Version 9.8)
- Ours: Version R2020a with KMUTT license
- Software program for numerical computations
  - Simple arithmetic and function calculations
  - Vectors and matrix manipulations

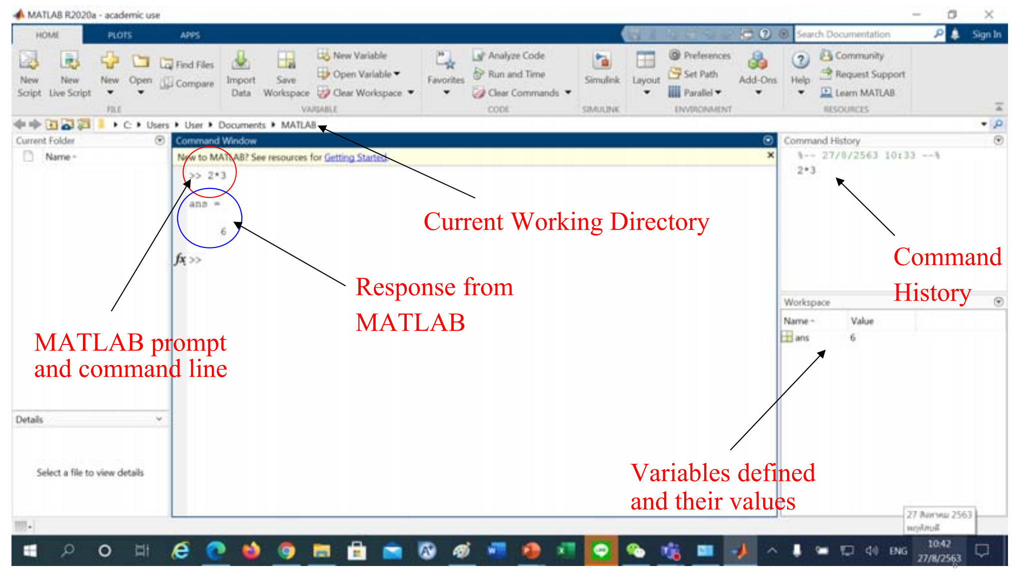
What Is MATLAB? (Cont'd)

- Equations solving
  1. Linear algebraic equations
  2. Nonlinear algebraic equations
  3. Ordinary differential equations (ODEs)
  4. Partial differential equations (PDEs)
- Programming
- Plotting

Getting Started

- On PCs, click on the MATLAB icon in Desktop
- Terminating a MATLAB session:
  1. Click on the "Close Window" button
  2. Select Exit MATLAB from the File pulldown menu
  3. Press Cntrl+Q on the command line
  4. Type exit or quit at the command line
  5. Cntrl+C will interrupt a MATLAB task but will not exit the program

Getting Started (Cont'd)



Getting Help in MATLAB

- Very extensive set of help at the command line:

demo	Opens Help browser to MATLAB examples
help *topic*	Display on-line help on a topic (with syntax and examples) at command line Type help to view all topics
doc helpwin help	Online help and comprehensive hypertext documentation and trouble-shooting

Lookfor vs. Help

- The lookfor command searches for functions based on a keyword in the first line of help text
- For example, MATLAB does not have a function named "inverse":

  >> help inverse

  inverse.m not found. => response from MATLAB

  >> lookfor inverse => will find many matches

Simple Arithmetic Capabilities

```
>> clc          % Clear the screen
>> clear        % Clear all the variables in session
>> 2 + 3        % Simple addition
ans =
    5

>> 2*3          % Simple multiplication
ans =
    6
```


Simple Arithmetic Capabilities (Cont'd)

```
>> 3 / 6          % Simple division
>> 2^3            % Exponentiation of power
>> 10 / (3+2)     % More complex expression
ans =
    2
```

Arithmetic Operators:

+	Addition	/	Division
-	Subtraction	\	Left division
*	Multiplication	^	Power
( )	Specify evaluation order by the degree of nesting		

Other Tidbits

```
>> 6 / 3 , 3 \ 6      % Use , to execute more than 1 operation
ans =
    2
ans =
    2
```

The semicolon ; will suppress the output but save the result

```
>> 2+3 ;    %Will produce no output but save the result in ans
>> ans      % Retrieve the result
ans =
    5
```


Other Tidbits (Cont'd)

- Use up-arrow to recall previously entered commands ↑
- A statement can be continued onto the next line with

  3 or more periods followed by a return

```
>> 2 + 3 ...      % Use 3 periods to continue the next line
+ 10
ans =
    15
```

Input and Output Format for Numbers

- All computations in MATLAB are done in double precision (16 digits)
- Uses conventional decimal notation
- Scientific notation uses the letter *e* to specify a power-of-ten scale factor
- Imaginary numbers use either *i* or *j* as a suffix

Input and Output Format for Numbers

- Examples of legal numbers are:

3	-99	0.0001
9.6397238	1.60210e-20	6.02252e25
1i	-3.14159j	3e5i

- Format command is used to switch between different display formats.

Display Output for Numbers with Format

>> format	% Default. Same as “format short”
>> format short	% Scaled fixed point format with 5 digits
>> format long	% Scaled fixed point format with 15 digits
>> format shorte	% Floating point format with 5 digits
>> format longe	% Floating point format with 15 digits
>> format shorteng	% Engineering format that has at least 5 digits and a power that is a multiple of three
>> format longeng	% Engineering format that has exactly 16 significant digits and a power that is a multiple of three
>> format compact	% Suppresses extra line-feeds
>> format loose	% Puts the extra line-fees back in

Display Output for Numbers with Format

```
>> pi                  % Display value of pi using default format
ans =
     3.1416

>> format long, pi     % Long, fixed format pi
ans =
     3.14159265358979
>> format shorte, pi            % Short, scientific notation for pi
ans =
    3.1416e+00
```

Use fprintf command to write formatted data to file or screen

Syntax: fprintf (fid, format, A, ……)

The fprintf Command

Syntax: fprintf (fid, format, A, ……)

where fid = output filename; if blank, output is screen
format = format control of data
A = variable name (e.g. vector, matrix, etc.)

```
>> A = pi;
>> fprintf ('%10.6f', A)    % print value of pi in fixed point
                            % format with a maximum of 10
                            % characters and 6 decimal places
3.141593
```


The fprintf Command (Cont'd)

```
>> A = pi;, B =2*pi;
>> fprintf ('%10.6f', A, B)
3.141593  6.283185

>> fprintf ('%10.6f\n', A, B)        % \n forces a new line in output
3.141593
6.283185
```

Type 'help fprintf' to view more information about the the command and how to write to an output file.
Another useful command to display output is disp(x), where x could be an array or a string enclosed in ' '. The command displays the array without printing the array name.

Predefined Variables

ans	The most recent answer
i, j	Imaginary unit
pi	The value of *pi* (3.141592653)
Inf	Infinity
NaN	Not-a-Number (i.e. 0/0 or Infinity/Infinity)

Built-in Mathematical Functions

- MATLAB has many built-in mathematical functions
- Type "help elfun" and "help specfun" for a list of functions
- Some common ones are:

abs(x)	Gives the absolute value of x
sqrt(x)	Gives the square root of x
exp(x)	Exponential of x
log(x)	Natural logarithm of x
log10(x)	Logarithm to the base 10 of x

Built-in Mathematical Functions (Cont'd)

sin(x)	Sine of x, for x in radians
asin(x)	Arcsin(x)
csc(x)	Produces 1/sin(x)
round(x)	Gives the integer closest to x
real(x)	Gives the real part of a complex number

```
>> x = exp(1)            % Numerical value of e
x =
   2.7183
```


An Example

```
%
% Here is a simple sequence of expressions to compute
% the volume of a cylinder, given its radius and length.
%
>> radius = 2;                        % radius of cylinder
>> length = 4;                        % length of cylinder
>> volume = pi*radius^2*length        % volume of cylinder
volume =
   50.2655
```


Writing a MATLAB Script File

- A script is an external text file containing a sequence of MATLAB statements.
  - Has the file extension .m
  - Very useful for running MATLAB non-interactively by executing many MATLAB statements with one Enter keystroke by typing the script filename.
  - The first character of the file name must be an alphabet, but the file name may contain numerals.
  - Must make sure the file name does not coincide with built-in MATLAB function names, e.g. sum, sin, mean.

Writing a MATLAB Script File (Cont'd)

- Two simple ways to create a MATLAB script file:
  1. Use a text editor in Windows or use the built-in Editor in MATLAB by choosing New Script in the ribbon.
  2. Use MATLAB *diary* command to record an interactive session.

     ```
     >> diary filename
     >> (some MATLAB commands)
     >> (some MATLAB output)
     >> diary off
     ```

     Then edit the file to delete MATLAB output, including incorrect commands and any error messages. Save the file again with the extension .m.

Example of a Script File

- Create a script file named "Volume.m"

```
clear
clc
radius = 2;
length = 4;
volume = pi*radius^2*length;
fprintf ('The volume of the cylinder = %4.2f \n', volume)
```

- Notice that the file name of a script is case-sensitive.
- Also, you are not allowed to use the same name for a variable in the script and the script file name.

Vector and Matrix Manipulations

Matrices and Vectors

Vectors and One-Dimensional Arrays

1. Row Vector

```
>> a = [1 3 9 25 1]          % Syntax for a row vector with
                             % elements separated by a space
>> a = [1, 3, 9, 25, 1]      % Syntax for a row vector with
                             % elements separated by a comma
a =
     1     3     9    25     1
```


Matrices and Vectors (Cont'd)

2. Column Vector

```
>> b = [1; 3; 2; 5]    % Syntax for a column vector with
                       % elements separated by a semicolon
b =
     1
     3
     2
     5
```

Some Vector Operations/Manipulations

>> a(2) % Determine the value of the 2nd element of the vector

ans =

3

>> length(a) % Determine the number of elements in vector

ans =

5

>> a(7) = 49 % Add an additional element to the vector a

a =

1 3 9 25 1 0 49

Some Vector Operations/Manipulations

>> a(6) = 16 % Change the 6th element of the vector

a =

1 3 9 25 1 16 49

Many of the functions introduced can be applied to a vector

>> sqrt(a) % Determine the square root of each element

ans =

1.0000 1.7321 3.0000 5.0000 1.0000
4.0000 7.0000

Other useful functions are:

min(a), max(a), mean(a), median(a)

Some Vector Operations/Manipulations

>> c = [2 4 5 3]’ % c is the transpose of the row vector

c =

2
4
5
3

>> 3*b – c % array operations can be performed on each element

ans =

1
5
1
12

Some Vector Operations/Manipulations

Arrays can be combined

>> [c ; b] % Join two column vectors to form a new one

ans =

2
4
5
3
1
3
2
5

Some Vector Operations/Manipulations

When division, exponentiation, or other operators are involved, the syntax is to put a period '.' before the operator without any spacing:

```
>> a./2          % Divide each array element by 2
ans =
    0.5000    1.5000    4.5000    12.5000    0.5000
8.0000    24.5000
```

```
>> b'.*c'        % Form product of the individual elements,
```
i.e. $[b_1c_1, b_2c_2, \ldots, b_nc_n]$

```
ans =
    2    12    10    15
```


Some Vector Operations/Manipulations

```
>> (b'.*c').^2        % Another example of exponentiation and .
ans =
    4    144    100    225
```

Vector inner and outer products:

```
>> c'*b       % Form inner product of 2 vectors → a scalar
ans =
    39
```


Some Vector Operations/Manipulations

```
>> b*c'      % Form the outer product of 2 vectors → a matrix
ans =
     2     4     5     3
     6    12    15     9
     4     8    10     6
    10    20    25    15
```

Matrices:

Some basic conventions:

1. Separate the element of a row with a blanks or commas

Matrices (Cont'd)

2. Use semicolons ; to indicate the end of each row
3. Surround the entire list of elements with square brackets, [ ]

```
>> A = [1 2 3; 5 7 4]          % Entering a 2×3 matrix
A =
     1     2     3
     5     7     4

>> A(2,1)     % Access element of second row, first column
ans =
     5
```

Matrices (Cont'd)

Consider a larger matrix:

>> B = [2 3 1 5 7; 3 5 1 6 7; 8 3 2 1 4; 5 7 10 3 4]

B =

2	3	1	5	7
3	5	1	6	7
8	3	2	1	4
5	7	10	3	4

Sub-matrices can be extracted from B using the colon operator

The syntax is: (start_row:end_row, start_column:end_column)

Matrices (Cont'd)

>> B_submatrix = B(2:3, 2:4) % Extract a 2×3 sub-matrix

B_submatrix =

5	1	6
3	2	1

>> A(:, 3) = [ ] % Delete the third column of matrix A

A =

1	2
5	7

>> A(:, 3) = [3; 4] % Add another column to A

A =

1	2	3
5	7	4

Matrices (Cont'd)

Some useful functions for manipulating matrices:

diag(A) - Produces the diagonal of matrix A

inv(A) - Finds the inverse of matrix A

eig(A) - Computes the eigenvalues of matrix A

eye(n) - Generates an $n \times n$ identity matrix

zeros(n, m) - Generates an $n \times m$ matrix of zeros

ones(n, m) - Generates an $n \times m$ matrix of ones

Matrix manipulations can be used to solve a system of algebraic equations!!!

Example of the Use of Matrices

To solve a Stoichiometric Balance Problem:

$$x_1 CH_4 + x_2 O_2 \dashrightarrow x_3 CO_2 + x_4 H_2O \quad \text{(combustion of methane)}$$

The balance equations are:

$$x_1 = x_3 \;,\; 4x_1 = 2x_4 \;,\; 2x_2 = 2x_3 + x_4$$

3 equations but 4 unknowns ==> set $x_1 = 1$

Example of the Use of Matrices (Cont'd)

The matrix form is:

$$\begin{pmatrix} 1 & 0 & -1 & 0 \\ 4 & 0 & 0 & -2 \\ 0 & 2 & -2 & -1 \\ 1 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

The solution from MATLAB is:

$CH_4 + 2O_2 \dashrightarrow CO_2 + 2H_2O$

Solving Nonlinear Algebraic Equations

Solving Nonlinear Equations

❑ There are 3 important MATLAB functions for solving nonlinear equations: $f(\underline{x}) = 0$

1. roots → special function to solve for polynomial roots
2. solve →generalized *symbolic* solver for roots of a set of nonlinear equations
3. fsolve → generalized *numerical* solver for roots of a set of nonlinear equations

Syntax of Roots Function

❑ Syntax of roots is:

ROOTS(*C*) computes the roots of the polynomial whose coefficients are the elements of the vector *C*.

If *C* has N+1 components, the polynomial is *C*(1)**X*^N + *C*(2)**X*^(N-1) + ... + *C*(N)**X* + *C*(N+1).

Example of Using Roots

Solve the following polynomial equation:

$$3x^4 + 2x^3 + x^2 + 4x - 6 = 0$$

```
>> c = [3 2 1 4 -6];
>> roots(c)
ans =
 -1.5476
  0.0435 + 1.2750i
  0.0435 - 1.2750i
  0.7940
```


Syntax of the Function Solve

- The solve function can be used to solve nonlinear algebraic equations either symbolically or numerically if no analytical solution is available.

The most widely used syntax is (see help too):

solve(eqn1, eqn2, …, eqnN)

solve(eqn1, eqn2, …, eqnN, var1, var2, …, varN)

Some Examples of Using Solve

```
>> syms a b c x
>> solve (a*x^2+b*x+c==0, x)        % Produce an analytical
                                       solution
ans =
 -(b + (b^2 - 4*a*c)^(1/2))/(2*a)
 -(b - (b^2 - 4*a*c)^(1/2))/(2*a)

>> syms x
>> solve(x-cos(x)==0)            % Produce a numerical result, or
>> solve(x==cos(x))

ans =

0.73908513321516064165531208767387
```


More Examples of Using Solve

Consider the following set of nonlinear equations:

$$x^2 + x - y^2 = 1 \quad \text{and} \quad y - \sin(x^2) = 0$$

```
>> syms x y
>> xy = solve (x^2+x-y^2-1==0, y – sin(x^2)==0)
xy =
 struct with fields:
   x: [1×1 sym]
   y: [1×1 sym]
>> xy.x
ans =
0.90908536662905988691187687185816

>> xy.y
ans =
0.73552157044815211836599760477997
```

```
[x y] = solve(…..)
x =
0.909085…

y =
0.735521…
```

Using the Double Command

- DOUBLE(X) returns the double precision value for X. If X is already a double precision array, DOUBLE has no effect.
- DOUBLE is very useful in converting symbolic numbers into double-precision numbers.

```
>> format short
>> syms x
>> z = solve(3*x^2-4*x-10==0)
 z =
 2/3 - 34^(1/2)/3
 34^(1/2)/3 + 2/3
>> double(z)
 ans =
   -1.2770
    2.6103
```

```
% Combine commands: disp + double
disp(double(xy.x))
      0.9091
              disp(double(xy.y))
      0.7355

% or if using [x y] = solve(…..)
 double(x)
double(y)
```


Specifying equations outside *Solve*

- Another way to use *Solve*? First just one unknown:

```
>> a = 4;
>> b = a/2;
>> syms x                    % define a symbolic variable
>> F = a*x-b*cos(x);
>> answer = solve(F);
>> disp(double(answer))
    0.4502
```


Using Parameters in Solve Function

- Now solve for 2 unknowns from 2 nonlinear equations:

```
% Solve a*y-cos(z)=0 and y+b*log(z) = 0
>> syms y z
>> F1 = a*y-cos(z);
>> F2 = y+b*log(z);
>> yz = solve(F1, F2);
>> disp(double(yz.y)), disp(double(yz.z))
    0.1499
    0.9278
```


Syntax of The Function fsolve

- The fsolve function solves a system of nonlinear equations of several variables.
- The most widely used syntax is (see help too):

  x = fsolve(fun, x0)

  where

  fun = an M-file function containing the system of nonlinear equations

  x0 = the initial guesses of the variables

Example of Using fsolve

- Solve: $2x_1 - x_2 - \exp(-x_1) = 0$ and $-x_1 + 2x_2 - \exp(-x_2) = 0$ starting at $x_1 = -5$ and $x_2 = -5$
- First, write an M-file that computes F, the values of the equations at x.

```
function F = myfun(x)
F = [2*x(1) - x(2) - exp(-x(1)); -x(1) + 2*x(2) - exp(-x(2))];
>> x0 = [-5 -5];
>> x = fsolve(@myfun, x0)
x =
     0.5671    0.5671
```


Solving Ordinary Differential Equations

Solving ODEs in MATLAB

- The most widely used functions in MATLAB to solve a system of 1st-order ODEs are: ODE23 and ODE45

$$dy/dt = f(t, y) \qquad \text{s.t. } y(0) = a$$

- Based on the Runge-Kutta numerical method
- ODE23 is low-order while ODE45 is medium-order
- The higher the order, the more accurate the numerical algorithm

Solving ODEs in MATLAB (Cont'd)

- A function is written for the ODEs as an M-file.

Example: Solve the following ODEs

$$dy_1/dt = 2y_1 - 0.001y_1y_2$$

$$dy_2/dt = -10y_2 + 0.002y_1y_2$$

$$\text{s.t. } y_1(0) = 5000$$
$$y_2(0) = 100$$

Solving ODEs in MATLAB (Cont'd)

- The syntax of ODE23 and ODE45 is:

  [t, y] = ode23(odefun, tspan, y0)

where odefun is the name of the M-file containing the ODE functions; tspan is the length of simulation; y0 is the initial condition

Create an M-file called 'fxy.m', which contains the following code:

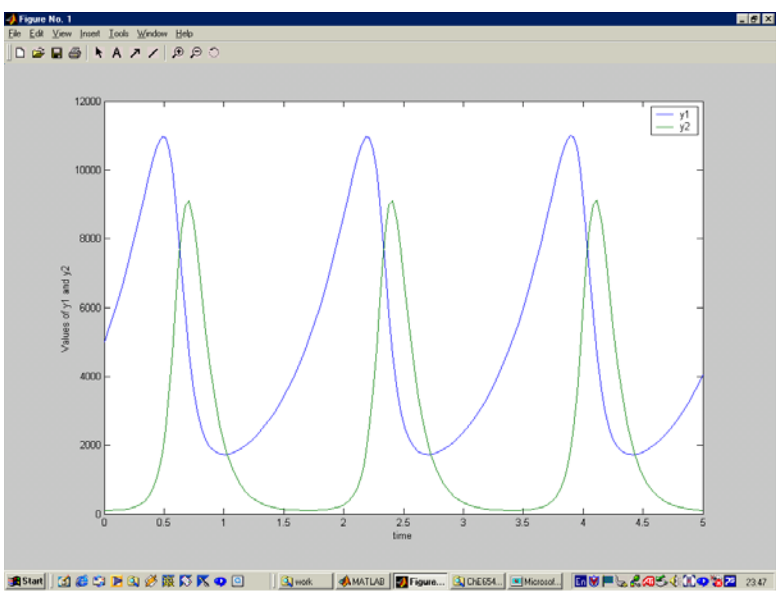
```
function fy = ode(t, y)
fy = zeros(2,1);        % Initialize fy as 2 × 1 matrix to zeros
fy(1) = 2*y(1)-0.001*y(1)*y(2);
fy(2) = -10*y(2)+0.002*y(1)*y(2);
```


Solving ODEs in MATLAB (Cont'd)

The solution of the ODEs can now be obtained by entering the following MATLAB commands, or put them into a script file:

```
>> simtime = 5;                  % Length of simulation
>> inity = [5000, 100];          % Initial values at t=0
>> [t, y] = ode23('fxy', simtime, inity)       % Solve the ODEs
>> plot(t,y);
>> xlabel('time')
>> ylabel('Values of y1 and y2')
>> legend('y1', 'y2')
```


Solving ODEs in MATLAB (Cont'd)



Plotting in MATLAB

MATLAB has extensive facilities for displaying vectors and matrices as graph, as well as annotating and printing these graphs.

```
>> x = [0 1 2 3 4 5 6 7 8 9 10];     % Setting the x values
>> y = x.^2;                          % y = x^2
>> plot(x,y)                          % Plot of a quadratic
>> title('Graph of a Quadratic')      % Put in a title for the graph
>> xlabel('Values of x')              % Label the x-axis
>> ylabel('y = x^2')                  % Label the y-axis
>> legend('y')                        % Put in a legend for multiple lines
```

Solving Higher-Order ODEs

- For higher-order ODEs (e.g. 2nd-order, 3rd-order, etc.), must reduce them to a system of 1st-order ODEs.

- There are 2 kinds of higher-order ODE problems:
  - Initial-value problems (IVPs)
  - Boundary-value problems (BVPs)

$y'' + 3y' - xy = \sin(x)$, $\quad y'(0) = 0, y(0) = 1$ $\quad$ => IVP

$y'' - xy' + y = \exp(-x)$, $\quad y'(0) = 0, y(1) = 2$ $\quad$ => BVP

$y''' + y'' + 3y' - y = 0$, $\quad y''(0) = 0, y'(0) = 1, y(2) = 5$ $\quad$ => BVP

Reducing Higher-Order ODEs

- Consider the 2nd order ODE:

$$d^2y/dt^2 = 3\, dy/dt + 6\, y - \cos(t), \qquad y'(0) = 0, y(0) = 1$$

The ODE can be converted into a pair of 1st-order ODEs:

Define $x = dy/dt$ so that

$$dx/dt = 3\, x + 6\, y - \cos(t) \qquad (1)$$

$$dy/dt = x \qquad (2)$$

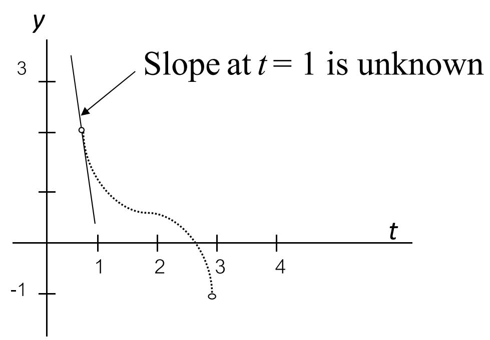
subject to $x(0) = 0, y(0) = 1$

Solving Boundary-Value Problems

- Shooting Method - Trial and Error

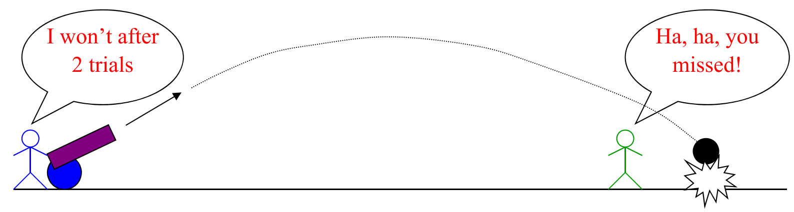
Consider the following 2nd-order ODE:

$$d^2y/dt^2 - (1 - t/5)\, y = t, \qquad y(1) = 2, y(3) = -1$$



Shooting Method (Cont'd)

- Based on the mechanics of an artillery problem



- Solve the ODE as an IVP by guessing the slope $y'(1)$ to get $y(3)$.

- If $y(3) > -1$, then the guess is too high. Guess a lower value for y'.

- If $y(3) < -1$, then the guess is too low. Guess a higher value for y'.

- After 2 trials, linearly interpolate or extrapolate for a third trial.

Shooting Method (Cont'd)

- The formula for linear interpolation/extrapolation is:

$$y'(1) = \text{G1} + \frac{\text{G2} - \text{G1}}{\text{R2} - \text{R1}}(\text{D} - \text{R1})$$

where G1 = first guess at initial slope
G2 = second guess at initial slope
R1 = first result at endpoint (using G1)
R2 = second result at endpoint (using G2)
D = desired value at the endpoint

<u>Note</u>: The third trial always gives the correct results if the ODE is *linear* => An ODE is linear if the coefficients of each derivative term and the forcing function are not functions of y.

Shooting Method in MATLAB

- First reduce the 2nd-order ODE into a pair of 1st-order ODEs:

$dy/dt = x$ and $dx/dt - (1- t/5)\,y = t$, $y(1) = 2, y(3) = -1$

- MATLAB m-file: fshoot.m

```
function fy = ode(t, y)
fy = zeros(2,1);
fy(1) = y(2);
fy(2) = (1-t/5)*y(1) + t;
```


Shooting Method in MATLAB (Cont'd)

- First trial => guess $y'(1) = x(1) = -1.5$

```
clc
clear
simtime = [1:0.2:3];
inity = [2, -1.5];
[t, y] = ode45('fshoot', simtime, inity);
```

Run from **t** = 1 to **t** = 3 with Δ**t** = 0.2

y **x** or **y′**

```
2.0000   -1.5000
1.7514   -0.9886
1.6043   -0.4814
1.5597    0.0389
1.6218    0.5876
1.7976    1.1783
2.0967    1.8227
2.5309    2.5310
3.1139    3.3116
3.8608    4.1706
4.7876    5.1119
```

y(**t**=3) which is > -1.0 wanted
so **y′**(1) is too large

Shooting Method in MATLAB (Cont'd)

- Second trial => guess $y'(1) = x(1) = -3.0$

```
clc
clear
simtime = [1:0.2:3];
inity = [2, -3.0];
[t, y] = ode45('fshoot', simtime, inity);
```

Run from **t** = 1 to **t** = 3 with Δ**t** = 0.2

y **x** or **y′**

```
2.0000   -3.0000
1.4498   -2.5118
0.9921   -2.0719
0.6192   -1.6598
0.3275   -1.2580
0.1163   -0.8512
-0.0118  -0.4259
-0.0520   0.0299
0.0029    0.5266
0.1620    1.0732
0.4360    1.6773
```

y(**t**=3) is > -1.0
so **y′**(1) is still too large

The Complete MATLAB File

```
% Shooting Method to solve a 2nd-order ODE
clc
clear
% first trial
simtime = [1:0.2:3];
g1 = -1.5;
inity = [2, g1];
[t, y] = ode45['fshoot', simtime, inity)
r1 = y(11,1);
% second trial
g2 = -3.0;
inity = [2, g2];
[t, y] = ode45('fshoot', simtime, inity)
r2 = y(11,1);
% third trial and the solution
g3 = g1 + (g2-g1)/(r2-r1)*(-1-r1);
inity = [2, g3];
[t, y] = ode45('fshoot', simtime, inity)
```

Output:

```
2.0000  -3.4950
1.3503  -3.0145
0.7900  -2.5967
0.3088  -2.2204
-0.0997  -1.8671
-0.4385  -1.5209
-0.7076  -1.1679
-0.9043  -0.7955
-1.0237  -0.3925
-1.0586   0.0511
-1.0000   0.5439
```

y(t=3)

Programming in MATLAB

Programming in MATLAB

- MATLAB is both a powerful programming language as well as an interactive computational environment

- Files that contain code in the MATLAB language are called M-files (file names must end with the extension '.m')

- There are 2 kinds of M-files:
  - Scripts, a simple text file where you can place MATLAB commands.
  - Functions, which can accept input arguments and return output arguments

The IF Condition Statement

- The IF statement evaluates a logical expression and executes a group of statements when the expression is true.

The general form of the IF statement is

```
IF expression
    statements
ELSEIF expression
    statements
ELSE
    statements
END
```

The ELSEIF and ELSE parts are optional. The valid operators in the expression are = =, <, < =, >, > =, and ~=.

Example of IF Condition Statements

Given a positive integer number, determine if the number is divisible by 5.

The m-file is called "ifthenelse"

```
clc
clear
number = input('Please enter a positive integer number: ')
if number < 0
        fprintf ('Sorry, %5i is not a positive number \n', number)
elseif round(number) - number ~= 0
        fprintf ('Sorry, %10.5f is not an integer number \n', number)
elseif rem(number, 5) == 0
        fprintf ('%5i is divisible by 5 \n', number)
else
        fprintf ('%5i is not divisible by 5 \n', number)
        remainder = rem(number,5);
        fprintf ('%5i is the remainder \n', remainder)
end
```

Returns the remainder if not divisible by 5

Example of IF Statements (Cont'd)

In MATLAB, type: ifthenelse

```
Please enter a positive integer number: -25
Sorry,   -25 is not a positive number
>>
Please enter a positive integer number: 15.23
Sorry,   15.23000 is not an integer number
>>
Please enter a positive integer number: 80
   80 is divisible by 5
>>
Please enter a positive integer number: 34
   34 is not divisible by 5
    4 is the remainder
>>
```


The FOR Statement

- The FOR statement repeats a group of statements a fixed, predetermined number of times.

The general form of the FOR statement is

```
FOR variable = expr
    statements
END
```

where expr is often of the form X:Y

Example of FOR Loop Statements

Given a positive integer number *n*, calculate the sum of (1+2+3+…+*n*)

The m-file is called "forloop"

```
clc
clear
number = input('Please enter a positive integer number: ')
if number < 0
   fprintf ('Sorry, %5i is not a positive number \n', number)
else
   sum = 0;
   for i = 1:number
            sum = sum + i;
   end
   fprintf ('The sum is  %8i \n', sum)
end
```

```
In MATLAB, type: forloop
Please enter a positive integer number: 100
The sum is     5050
>>
```

The WHILE and BREAK Statements

- The WHILE loop repeats a group of statements an indefinite number of times, under control of a logical condition.

The general form of the WHILE statement is

```
WHILE expression
    statements
END
```

- The BREAK statement lets you exit early from a FOR or WHILE loop. This prevents MATLAB from going into an infinite loop.

Example of WHILE Statements

The Hi-Lo game:

Objective: Try to correctly guess an integer between 0 and 100 generated by the computer in as few trials as possible.

The m-file is called "whileloop"

```
clc
clear
myinteger = round(100*rand);
flag = 0;
while flag ==0
    fprintf ('\n')
    guess = input('Please guess an integer between 0 and 100 I have in mind: ');
```


Example of WHILE Statements (Cont'd)

```
    if guess == myinteger
        flag = 1;
        fprintf ('\n')
        fprintf ('You guessed right!!!\n')
        fprintf ('My number is %3i \n', myinteger)
    elseif guess < myinteger
        fprintf ('Your number is too low.  Please guess again\n')
    else
        fprintf ('Your number is too high.  Please guess again\n')
    end
end
```


Example of WHILE Statements (Cont'd)

```
Please guess an integer between 0 and 100 I have in mind: 50
Your number is too low.  Please guess again

Please guess an integer between 0 and 100 I have in mind: 75
Your number is too low.  Please guess again

Please guess an integer between 0 and 100 I have in mind: 88
Your number is too high.  Please guess again

Please guess an integer between 0 and 100 I have in mind: 82
Your number is too high.  Please guess again

Please guess an integer between 0 and 100 I have in mind: 79
Your number is too low.  Please guess again

Please guess an integer between 0 and 100 I have in mind: 81

You guessed right!!!
My number is  81
>>
```

Workshops

Workshop 1: Basic Calculations

Use MATLAB to carry out the following calculations:

(a) Solve the equation: $2x^2 - 5x - 20 = 0$, using the quadratic formula. Report your answers in 6 decimal places.

(b) What is the product of the two roots of the quadratic equation: $4x^2 + 3x + 13 = 0$. Report your answer in 4 decimal places.

(c) Compute the distance between two points, namely (2, -4, 9) and (-3, 1, -7), given in the Cartesian coordinates.

(d) Convert the Cartesian coordinates (4, 15) into the polar coordinates (r, θ). Report your answers in 2 decimal places and show θ in both degree and radian.

Workshop 1: Basic Calculations (Cont'd)

Use MATLAB to carry out the following calculations:

(e) A quick search on the Internet shows that the vapor pressure of acetone is given by:

$$\log_{10}(P^{\mathrm{VAP}}) = 7.2316 - \frac{1277.03}{T + 237.23} \qquad \textbf{T} \text{ in } ^{\circ}\text{C and } \textbf{P} \text{ in mmHg}$$

Verify the accuracy of this vapor pressure at $T = 25$ °C by comparing it (in terms of relative % error with 5 decimal places) with the following vapor pressure equation reported by Ambrose, Sprake, *et al.* (1974):

$$\log_{10}(P^{\mathrm{VAP}}) = 4.42448 - \frac{1312.253}{T - 32.445} \qquad \textbf{T} \text{ in Kelvin and } \textbf{P} \text{ in bar}$$

Workshop 2: Matrix Manipulations

(a) Consider the following arrays:

$$\mathbf{A} = \begin{pmatrix} 1 & 4 & 2 \\ 2 & 4 & 100 \\ 7 & 9 & 7 \\ 3 & \pi & 42 \end{pmatrix} \qquad \mathbf{B} = \ln(\mathbf{A})$$

Use MATLAB to do the following (use "format short"):

- Select just the second row of **B**.
- Determine the sum of the second row of **B**.
- Multiply the second column of **B** and the first column of **A** (element-by-element)
- Determine the maximum value in the vector resulting from element-by-element multiplication of the second column of **B** with the first column of **A**.
- Determine the sum of the first row of **A** divided element-by-element by the first three elements of the third column of **B**.

Workshop 2 (Cont'd)

(b) Use MATLAB to determine the stoichiometric ratios of molecular species in the following reaction. You must find the lowest integer number for each stoichiometric coefficient.

$$a\ HIO_3 + b\ FeI_2 + c\ HCl \rightarrow d\ FeCl_3 + e\ ICl + f\ H_2O$$

where HIO_3 = Iodic Acid, FeI_2 = Ferrous Iodide,
$FeCl_3$ = Ferric Chloride, and ICl = Idodine Monochloride

Answers:

a = ______ b = ______ c = ______ d = ______
e = ______ f = ______

Workshop 3: Molar Volume and Z from Redlich-Kwong-Soave Equation of State

The Redlich-Kwong-Soave equation of state contains 2 empirical parameters a and b, and is given by:

$$P = \frac{RT}{\underline{V} - b} - \frac{a}{\underline{V}(\underline{V} + b)} \quad \text{where}$$

$$a = 0.42747[R^2 T_C^2/P_C]\alpha(T)$$

$$b = 0.08664[R\,T_C/P_C]$$

$$\alpha(T) = [1 + m(1 - T_r^{1/2})]^2 \text{ and } T_r = T/T_C$$

$$m = 0.480 + 1.57w - 0.176w^2$$

$$w = -1.0 - \log10\,[P^{VAP}(T_r = 0.7)/P_C] = \text{Pitzer acentric factor}$$

Workshop 3: Molar Volume and Z from Redlich-Kwong-Soave Equation of State

The variables are defined by:

- **P** = pressure in atm
- **$\underline{V}$** = molar volume in L/gmole
- **T** = temperature in K
- **R** = gas constant (0.08206 atm-L/gmole-K)
- **T_C** = the critical temperature (405.5 K for ammonia)
- **P_C** = the critical pressure (111.3 atm for ammonia)
- **P^{VAP}** = vapor pressure (6.2 atm at T_r = 0.7 for ammonia)

Use MATLAB to answer the following questions:

(a) Calculate the molar volume and compressibility factor **Z** for gaseous ammonia at a pressure **P** = 56 atm and a temperature **T** = 450 K.

(b) Repeat the calculations for the following reduced pressures: P_r = 1, 2, 4, 10, and 20.

Workshop 4: Solving an ODE

Write a MATLAB script file to solve the following 4th-order ODE using ode23:

$$d^4y/dt^4 = y + 7.5\sin(2t) + 16\sin^2 t - 14\cos^2 t + t^3$$

$$\text{s.t. } y(0) = 0,\ dy(0)/dt = 3,\ d^2y(0)/dt^2 = 6,\ d^3y(0)/dt^3 = -8$$

The above ODE has an analytical solution of:

$$y(t) = c_1 e^t + c_2\sin(2t) - c_3\cos^2(t) + c_4 t^3$$

Workshop 4: Solving an ODE (Cont'd)

Make a plot of the numerical solution (y versus t) from MATLAB. Then, compare your MATLAB solution with the analytical solution below by reporting the relative % differences. Run the simulation from $t = 0$ to $t = 1$ with an increment of 0.1. Include 6 decimal places in reporting all your numbers.

Note: You must do all your work in MATLAB, which includes determining the constants c_1, c_2, c_3, and c_4 in the analytical solution.

Workshop 5: Newton's Method

Consider the following system of nonlinear equations:

$$f_1(x, y, z) = xyz - x^2 + y^2 - 1.34 = 0$$

$$f_2(x, y, z) = xy - z^2 - 0.09 = 0$$

$$f_3(x, y, z) = e^x - e^y + z - 0.41 = 0$$

Write a MATLAB program to do the following:

(a) Solve for the roots of the above equations using Newton's method. Use an initial guess of $(x, y, z) = (1, 1, 1)$. Accept the solution only when $|f_1|$, $|f_2|$, and $|f_3| \le 10^{-3}$.

Workshop 5: Newton's Method (Cont'd)

(b) Solve the equations again using the function *solve* in MATLAB.

(c) Compare the % relative errors between the values of x, y, and z obtained from Newton and from MATLAB. Report the errors with 5 decimal places.

Recall that the iterative formula for Newton's method is:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \boldsymbol{J}^{-1}(\mathbf{x}_k) * \mathbf{f}(\mathbf{x}_k)$$

where $\boldsymbol{J}^{-1}$ is the inverse of the Jacobian matrix, $\boldsymbol{J}$

$$\boldsymbol{J} = \left\{ \begin{array}{llll} \partial f_1/\partial x_1 & \partial f_1/\partial x_2 & \ldots & \partial f_1/\partial x_n \\ \partial f_2/\partial x_1 & \partial f_2/\partial x_2 & \ldots & \partial f_2/\partial x_n \\ \ldots\ldots & \ldots\ldots & \ldots\ldots & \\ \partial f_n/\partial x_1 & \partial f_n/\partial x_2 & \ldots & \partial f_n/\partial x_n \end{array} \right\}$$