Introduction to GNU Octave

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Outline

1. Introduction
2. Getting Started
3. Vectors and Matrices
4. Plotting Graphs
5. Loops and Conditions
6. File I/O
7. Functions
8. Scripting

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What is GNU Octave?

- Octave is a high-level language, primarily intended for numerical computations.
- It provides a convenient command line interface for solving linear and nonlinear problems numerically, and for performing other numerical experiments.
- It may also be used as a batch-oriented language.
- Octave is often viewed as a system for numerical computations with a language that is mostly compatible with Matlab, but that is available as free software under the GNU GPL, and that can replace it in many circumstances.

Tutorial Goals

- The goal of this tutorial is to provide a brief introduction to a few of the capabilities of GNU Octave.
- Most of the functionality of Matlab already exists in GNU Octave and octave can run most Matlab scripts.
- Matlab users should review differences between Matlab and GNU Octave before porting matlab scripts to octave. `http://en.wikibooks.org/wiki/MATLAB_Programming/Differences_between_Octave_and_MATLAB`

Requirements

- Users can install GNU Octave on their laptops and desktops.
- Mac OS X: `http://www.octave.org/wiki/index.php?title=Installing_MacOS_X_Bundle`
- Windows: `http://www.octave.org/wiki/index.php?title=Octave_for_Windows`
- Linux: Check repositories for your distribution
  1. openSuSE: `zypper in octave`
  2. Ubuntu: `apt-get install octave`
  3. Fedora: `yum install octave`
- LSU HPC & LONI: Add soft key +octave-3.0.3-intel-11.1 to your .soft file and resoft

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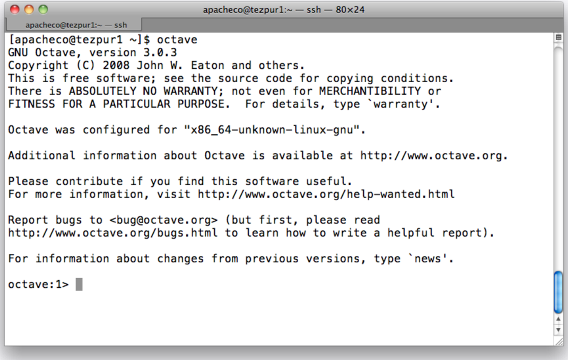
Getting Started

- Type `octave` in a terminal window (Linux, LSU HPC & LONI only)



```
[apacheco@tezpur1 ~]$ octave
GNU Octave, version 3.0.3
Copyright (C) 2008 John W. Eaton and others.
This is free software; see the source code for copying conditions.
There is ABSOLUTELY NO WARRANTY; not even for MERCHANTIBILITY or
FITNESS FOR A PARTICULAR PURPOSE.  For details, type `warranty'.

Octave was configured for "x86_64-unknown-linux-gnu".

Additional information about Octave is available at http://www.octave.org.

Please contribute if you find this software useful.
For more information, visit http://www.octave.org/help-wanted.html

Report bugs to <bug@octave.org> (but first, please read
http://www.octave.org/bugs.html to learn how to write a helpful report).

For information about changes from previous versions, type `news'.

octave:1> 
```

- The last line is the octave prompt
- You can also start octave with the -q option, octave information will not be printed

Entering Commands I

- Commands can be typed at the prompt or read from a script.
- Scripts are plain text files with file suffix `.m`.
- To run a script, type the script name without the suffix.
- “,” separates commands in a line and displays the output on the screen.
- To suppress output, use “;”.
- Comments are preceeded by %.
- Octave is case-sensitive.
- Getting Help:
  - `help` lists all built-in functions and internal variables.
  - `help name` explains the variable or function "name"

Entering Commands II

- Octave as a calculator:
  - Just type mathematical commands at the prompt.
  - Octave also has mathematical built-in functions.

Simple Arithmetic functions

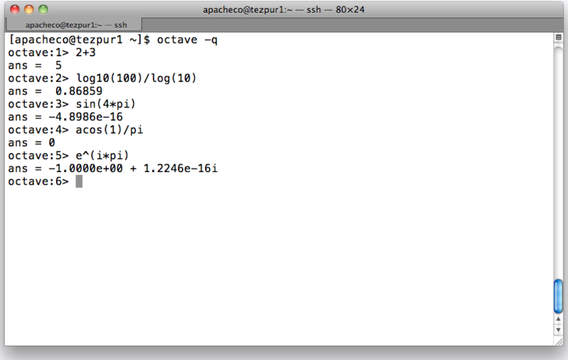
Addition:	+
Subtraction:	-
Multiplication:	*
Division:	/
Exponentiation:	**

Mathematical Functions

Trignometic Functions:	sin, cos, tan
Inverse Trignometric Functions:	asin, acos, atan
Logarithmic Functions:	log, log10
Exponentiation:	exp
Absolute value:	abs

- trignometric functions work in **radians**
- **pi, e, i** and **j** are predefined variables.
- **ans** variable is used to hold the result of the last operation.
- No need to declare variable or its type, variables are either **floating point** numbers or **strings**.
- To see the value of a variable, just type its name and hit return.

Entering Commands III



```
[apacheco@tezpur1 ~]$ octave -q
octave:1> 2+3
ans =  5
octave:2> log10(100)/log(10)
ans =  0.86859
octave:3> sin(4*pi)
ans = -4.8986e-16
octave:4> acos(1)/pi
ans = 0
octave:5> e^(i*pi)
ans = -1.0000e+00 + 1.2246e-16i
octave:6>
```

- Note that by default, octave prints variables with only 5 digits.
- At octave prompt, type `format long` to obtain variables with greater precision.

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Vectors

- Defining a Row Vector: $vr = (1\,2\,3)$

```
octave:1> vr = [1 2 3]
vr =

   1   2   3
```

- Defining a Column Vector: $vc = (vr)^T$

```
octave:2> vc = [1; 2; 3]
vc =

   1
   2
   3
```

- Autogeneration of Vector with constant increment: `Start:[increment]:End`

```
octave:3> a = 4:2:10
a =

    4    6    8   10
```

Matrices I

- A matrix $B = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix}$ is constructed as follows

```
octave:4> B = [1 2; 3 4]
B =

   1   2
   3   4
```

- Matrices can be assembled from submatrices

```
octave:5> b = 5:6
b =

  5  6
octave:6> A = [ B b’]
A =

   1   2   5
   3   4   6
```

*Matrices **II***

- Creating special matrices of size $m \times n$
  1. eye(m,n): Create a matrix with ones on the diagonal and zeros elsewhere. Identity matrix if $m = n$
  2. zeros(m,n): Create a null matrix
  3. ones(m,n): Create a matrix where all elements are 1
  4. rand(m,n): generates a random matrix whose entries are uniformly distributed in the interval (0,1).

```
octave:7> eye(3,2)
ans =

   1   0
   0   1
   0   0

octave:8> eye(3,3)
ans =

   1   0   0
   0   1   0
   0   0   1

octave:9> zeros(3,2)
ans =

   0   0
   0   0
   0   0
```

```
octave:10> ones(3,4)
ans =

   1   1   1   1
   1   1   1   1
   1   1   1   1

octave:11> rand(5,2)
ans =

   1.7700e-01   1.4495e-01
   7.5533e-01   7.9854e-01
   3.4831e-04   7.6881e-01
   5.6224e-01   1.0213e-01
   5.3236e-01   9.2427e-01
```

Matrices III

- Basis Arithmetic:
  - `+, - and *` denote matrix addition, subtraction and multiplication respectively.
  - `A'`: transpose and conjugates A
  - `A.'`: transposes A

```
octave:1> A = [1+i 2+2i;3-i 4-2i]
A =

   1 + 1i   2 + 2i
   3 - 1i   4 - 2i
octave:3> A+B,A*B
ans =

   3 + 1i   4 + 2i
   5 - 1i   6 - 2i

ans =

    6 +   6i    6 +   6i
   14 -   6i   14 -   6i
```

```
octave:2> B = 2*ones(2,2)
B =

   2   2
   2   2

octave:4> A',A.'
ans =

   1 - 1i   3 + 1i
   2 - 2i   4 + 2i

ans =

   1 + 1i   3 - 1i
   2 + 2i   4 - 2i
```

Matrices IV

- Element wise operations: Use `.{operator}` for element wise operation

```
octave:1> A = [ 1 2; 3 4]
A =

   1   2
   3   4

octave:2> A.**2
ans =

    1    4
    9   16
```

```
octave:3> B = [ 2 2; 6 4]
B =

   2   2
   6   4

octave:4> A./B
ans =

   0.50000   1.00000
   0.50000   1.00000
```

Matrices V

- Indexing and Slicing
  - $v(k)$: k^{th} element of vector v
  - $A(k,l)$: matrix element A_{kl}
  - $v(m:n)$: slice of vector v from element m through n
  - $A(k,:)$: k^{th} row of matrix A
  - $A(:,l)$: l^{th} column of matrix A
- `length(v)`: returns the number of elements of vector v
- `size(A)`: returns the number of rows and columns of matrix A

Linear Algebra I

- GNU Octave is capable of solving Linear Algebra problems
  1. Solving Ax = b
     Solve the equations $x + y = 3$ and $2x - 3y = 5$

```
octave:1> A = [ 1 1; 2 -3] , B = [3 5]’
A =

   1   1
   2  -3

B =

   3
   5

octave:2> A\B
ans =

   2.80000
   0.20000
```

```
octave:3> inv(A)*B
ans =

   2.80000
   0.20000

octave:4> A*(A\B)
ans =

   3
   5
```

- Calculate determinant of a matrix: `det(A)`
- Calculate inverse of a matrix: `inv(A)`

Linear Algebra II

- Calculate eigenvectors and eigenvalues of a matrix

```
octave:1> A = [1 2 3; 4 5 6; 7 8 9]
A =

   1   2   3
   4   5   6
   7   8   9

octave:2> eig(A)
ans =

   1.6117e+01
  -1.1168e+00
  -1.3037e-15
```

```
octave:3> [V,D] = eig(A)
V =

  -0.231971  -0.785830   0.408248
  -0.525322  -0.086751  -0.816497
  -0.818673   0.612328   0.408248

D =

Diagonal Matrix

   1.6117e+01            0            0
            0  -1.1168e+00            0
            0            0  -1.3037e-15
```

- To calculate eigenvectors, you need to provide two variables for the answer.
- Check if we can obtain A by evaluating $A = VDV^{-1}$

Linear Algebra III

- For non square matrix, Octave can also carry out Singular Value Decomposition (SVD)
- SVD takes a $m \times n$ matrix A and factors it into $A = USV^T$ where
  - U is a $m \times m$ orthogonal matrix whose columns are eigenvectors of AA^T
  - V is a $n \times n$ orthogonal matrix whose columns are eigenvectors of A^TA
  - S is a $m \times n$ diagonal matrix whose elements are the square roots of the eigenvalues of AA^T and A^TA

```
octave:1> A = [ 1 3 -2 3; 3 5 1 5; -2 1 4 2]
A =

   1   3  -2   3
   3   5   1   5
  -2   1   4   2

octave:2> svd(A)
ans =

   8.9310
   5.0412
   1.6801

octave:4> U*S*V'
ans =

   1.0000   3.0000  -2.0000   3.0000
   3.0000   5.0000   1.0000   5.0000
  -2.0000   1.0000   4.0000   2.0000
```

```
octave:3> [U,S,V] = svd(A,0)
U =

  -4.6734e-01   3.8640e-01   7.9516e-01
  -8.6205e-01   3.3920e-04  -5.0682e-01
  -1.9611e-01  -9.2233e-01   3.3294e-01

S =

   8.93102   0.00000   0.00000
   0.00000   5.04125   0.00000
   0.00000   0.00000   1.68010

V =

  -0.297983   0.442764  -0.828029
  -0.661559   0.047326   0.109729
  -0.079700  -0.885056  -0.455551
  -0.683516  -0.135631   0.307898
```

Other Linear Algebra Functions I

- `A/B` computes `X` such that `XB = A`.
- `A\B` computes `X` such that `AX = B`.
- `norm(A,p)` computes p-norm of the matrix (or vector) `A`, default is $p = 2$.
- `rank(A)` computes the numerical rank of matrix `A`.
- `trace(A)` computes the trace of a matrix `A`.
- `logm(A)` computes the matrix logarithm of a square matrix.
- `expm(A)` computes the matrix exponential of a square matrix.
- `sqrtm(A)` computes the matrix square root of a square matrix.
- `R = chol(A)` computes the Cholesky factorization of the symmetric definite matrix `A` such that $R^T R = A$
- `[L,U] = lu(A)` computes the LU decomposition of `A`, $A = LU$
- `[Q,R] = qr(A)` computes the QR decomposition of `A`, $A = QR$

Other Mathematical Function in Octave

- Numerical Integration
- Differential Equations
- Polynomial Manipulations
- Statistical Analysis
- Interpolation
- Signal and Image Processing
- Object Oriented Programming

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Plotting Graphs via GNUPLOT I

- Octave can plot graphs via the open-source program GNUPLOT
- If given just one pair of numbers, it plots a point.
- If given a pair of vectors, it plots all the points given by the two vectors.
- Usage:
  - `plot(x,y[,fmt])`: Plots a line through the points (x_i, y_i). Select line style and color with the `fmt` string.
  - `semilogx(x,y[,fmt])`: Plot with a logarithmic scale for the x-axis
  - `semilogy(x,y[,fmt])`: Plot with a logarithmic scale for the y-axis
  - `semilog(x,y[,fmt])`: Plot with a logarithmic scale on both axes

Plotting Graphs via GNUPLOT II

- Procedure for plotting 2D graphics: $y = f(x)$
  1. Generate a vector with the x-coordinates to be plotted.

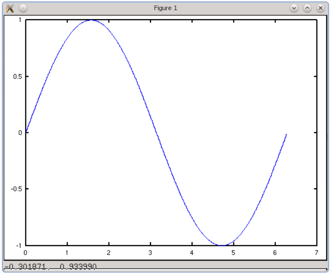
     ```
     octave:1> x = 0:0.01:2*pi;
     ```

  2. Generate a vector containing the corresponding y-values

     ```
     octave:2> y=sin(x);
     ```

  3. Use the plot command to plot $\sin(x)$

     ```
     octave:3> plot(x,y);
     ```



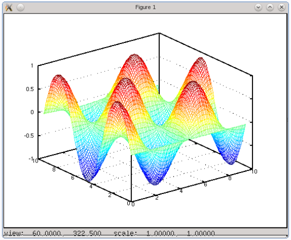
- Procedure for plotting 3D graphics

1. Generate a grid data for a 3D plot: Requires two matrices *xx* whose rows are copies of *x* and *yy* whose columns are copies of y

```
octave:1> x = 0:0.1:3*pi;
octave:2> y = 0:0.1:3*pi;
octave:3> [xx,yy]=meshgrid(x,y);
```

2. Plot a surface in 3D

```
octave:4> z = sin(x)'*cos(y);
octave:5> mesh(x,y,z);
```



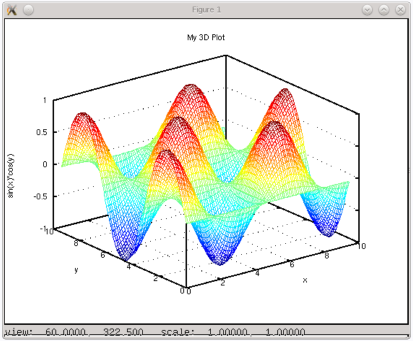
```
view:  60.0000,  322.500   scale:  1.00000,  1.00000
```

Commands for 2D and 3D graphics I

- `title(string)` writes `string` as title for the graphics
- `xlabel(string)` labels the $x-$axis with `string`
- `ylabel(string)` labels the $y-$axis with `string`
- `zlabel(string)` labels the $z-$axis with `string`
- `axis(v)` set axes limits for the plot. `v` is a vector of the form `v = (xmin,xmax,ymin,ymax[,zmin,zmax])`.
- `hold [on|off]` controls whether the next graphics output should or shouldn't clear the previous graphics.
- `clg` clears the graphics window.

*Commands for 2D and 3D graphics **II***

```
octave:6> title('My 3D Plot');
octave:7> xlabel('x');
octave:8> ylabel('y');
octave:9> zlabel('sin(x)*cos(y)');
```



```
view: 60.0000, 322.500 scale: 1.00000, 1.00000
```

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Control Statements I

- Control Statements such as `if, do, while` and so on control the flow of execution in Octave Programs.
- Each control statement has an `end` statement that marks the end of the control statement.

The IF Statement

The general form of the `IF` statement is

```
if (condition)
  then-body
elseif (condition)
  elseif-body
else
  else-body
endif
```

```
if (rem (x,2) == 0)
    printf (``x is even\n'');
elseif (rem (x,3) == 0)
    printf (``x is odd and divisible by 3\n'');
else
    printf (``x is odd\n'')
endif
```

The `elseif` and `else` blocks are optional

Control Statements II

The SWITCH Statement

The SWITCH statement is similar to the SELECT CASE statement in Fortran 90 and allows one to carry out different operation based on one variable.

```
switch expression
  case label
    command_list
  case label
    command_list
  otherwise
    command_list
endswitch
```

```
a = rem (y,2);
switch a
  case 0
    printf (‘‘x is even\n’’);
  otherwise
    b = rem (y,3);
    switch b
      case 0
        printf (‘‘x is odd and divisible by 3\n’’);
      otherwise
        printf (‘‘x is odd\n’’)
    endswitch
endswitch
```

Control Statements III

The WHILE Statement

The WHILE statement is the simplest form of a looping construct. It repeatedly executes a statement as long as a condition is true

```
while (condition)
  body
endwhile
```

```
fib = ones(1, 10);
i = 3;
while ( i <= 10 )
  fib(i) = fib(i-1) + fib(i-2);
  i++;
endwhile
```

Control Statements IV

The DO-UNTIL Statement

The DO−UNTIL statement is similar to the WHILE statement except that it repeatedly executes a statement until a condition is true. The test of the condition is at the end of the loop so that the loop executes at least once.

```
do
  body
until (condition)
```

```
fib = ones(1, 10);
i = 2;
do
  i++;
  fib(i) = fib(i-1) + fib(i-2)
until ( i == 10)
```

Control Statements V

The FOR Statement

The FOR statement makes it convenient to count iterations of a loop

```
for var = expression
  body
endfor
```

```
for I=1:N
  sumft=0;
  for J=1:M
    sumft=sumft+ftmwvels(I,J)^2;
  endfor
  fprintf(fid,’’ %15.8e  %21.14e\n’’,(I-1)*dw,sumft);
endfor
```

The BREAK and CONTINUE Statements

The BREAK statement allows you to jump from the inside of a loop past the end of a loop

The CONTINUE statement allows you to jump from the inside of a loop to the beginnng of the loop

The BREAK and CONTINUE can be used inside a for, while or do...until loop.

```
total = 0;
while true
   x = input('Value to add (enter 0 to stop): ');
   if x == 0
      break;
   endif
   total = total+x;
   disp(['Total: ', num2str(total)]);
endwhile

N = 5;
A = zeros(N); % Create an N x N matrix filled with 0s

for row = 1:N
   for column = 1:N
      if column > row
         continue;
      endif
      A(row, column) = 1;
   endfor
endfor
```

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Simple File I/O I

- `save` and `load` commands allow data to be written to and read from disk files in various formats.

```
apacheco-3:~ apacheco> octave -q
octave-3.2.3:1> A = [1 2 3; 4 5 6; 7 8 9];
octave-3.2.3:2> save myfile.mat A
octave-3.2.3:3>
apacheco-3:~ apacheco> cat myfile.mat
# Created by Octave 3.2.3, Fri Apr 13 12:53:36 2012 CDT <apacheco@apacheco-3.lsu.edu>
# name: A
# type: matrix
# rows: 3
# columns: 3
 1 2 3
 4 5 6
 7 8 9
apacheco-3:~ apacheco> octave -q
octave-3.2.3:1> load myfile.mat
octave-3.2.3:2> A
A =

   1   2   3
   4   5   6
   7   8   9
```

- Octave can save and read data in various formats such as ASCII, binary, MATLAB binary format, hdf5.

C style I/O Functions

- Octave C style input and output functions provides most of the functionality of C programming language's standard I/O library.
- Opening and Closing Files: When reading or writing data to a file, it must be opened first

```
fid = fopen(``water-hexamer-cage-bomd.ftmwvels'',''w'');
dw = 1/(N*deltat);
for I=[1:N]
  sumft=0;
  for J=[1:M]
    sumft=sumft+ftmwvels(I,J)^2;
  endfor
  fprintf(fid,'' %15.8e  %21.14e\n'',(I-1)*dw,sumft);
endfor
fclose(fid);
```

- Octave can open files in various modes, the above example is for writing.

r : Open a file for reading.
w : Open a file for writing.
a : Open or create a file for writing at the end of the file.
r+ : Open an existing file for reading and writing.
w+ : Open a file for reading and writing and discard previous contents.
a+ : Open or create a file for reading and writing at the end of the file.

Formatted Output

- Octave provides function for printed formatted output which are modelled on the C language functions.

  printf (template, . . .) : Print optional argumentsunder the control of string `template`.
  fprintf (fid, template, . . .) : Same as `printf` except that output is written to stream `fid` instead of `stdout`.
  sprintf (template, . . .) : Same as `printf` except that the output is returned as a string.

- Output Conversion Syntax:

  General Form: `% flags width [.precision] type conversion`

  %7d : Prints an integer with a width of 7.
  %8.3f : Prints a floating point number with a width of 8 and precision of 3.
  %11s : Prints a string of width 11.
  %21.14e : Prints a floating point number in exponential notation with a width of 21 and precision 14.

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Functions I

- Complicated Octave programs can be simplified by defining functions.
- In the simplest form, a function, `name`, is defined as follows:

```
function name (argument-list)
   body
endfunction
```

```
[apacheco@tezpur1 octave]$ cat hello.m
function hello (message)
   printf (‘‘%s\n’’,message)
endfunction
[apacheco@tezpur1 octave]$ octave -q
octave:1> hello (‘‘Hello World’’)
Hello World
```

- In some instances, your program may need some information back from the function that you have defined.
- Syntax for writing a function that returns
  1. a single value

     ```
     function ret-var = name (argument-list)
       body
     endfunction
     ```

  2. multiple values

     ```
     function [ret-list] = name (argument-list)
       body
     endfunction
     ```

Functions II

- The symbol `ret-var` is the name of the variable that will hold the value to be returned by the function.
- The symbol `ret-list` is a comma separated list of variables that will hold the values returned by the function.
- `ret-var` and `ret-list` must be defined before the end of the function body.
- Variables defined in the function including `ret-var, ret-list` and `argument-list` are local to the function.

```
v = rand(10,1);

function average = avg (a)
  average = sum(a)/length(a) ;
endfunction

function [max,id] = vmax(a)
  id = 1;
  max = a(id);
  for i = 2:length(a)
    if ( a(i) > max )
      max = a(i) ;
      id = i ;
    endif
  endfor
endfunction
```

```
b = rand(20,1);
[max,id] = vmax(b);
printf ( ``Average of vector v = %f\n'', avg(v))
printf ( ``Maximum value of vector b = %f with \
   id = %d\n'',max,id )
```

```
[apacheco@tezpur1 octave] ./func.sh
Average of vector v = 0.512198
Maximum value of vector b = 0.996040 with id = 7
```

Functions III

- Instead of defining functions each time you need them, you can save the function to a Function File and use them whenever needed.
- Function Files end with a `.m` extension with a prefix that matches the function name.
- Function files should contain only one function, see `hello.m` two slides back.
- When a function is called, octave searches a list of directory for a file that contains the function declaration.
- If the function file is not in the current directory, you can add the directory to search for the function file using the `addpath` command

  `addpath("~/Octave:~/Octave-Func")`: Add `~/Octave` and `~/Octave-Func` to the load path for searching function files.

Outline

1. Introduction
2. Getting Started
3. Vectors and Matrices
4. Plotting Graphs
5. Loops and Conditions
6. File I/O
7. Functions
8. Scripting

Script Files I

- A script file is a file containing any sequence of Octave commands.
- It is read and evaluated as if you have entered the commands interactively at the octave prompt.
- A script file must not begin with a function keyword. If the script file begins with a function keyword, Octave will assume that it is a function file and will evaluate only the function when it is called.
- Unlike a function file, variables in the script file are global and can be accessed by any line/command in the script.
- Octave normally executes commands from a script file with a `.m` extension.
- The `source` command allows Octave to execute commands from any file `source(file.exe)` to execute commands in the `file.exe` file.

Script Files II

```
[apacheco@tezpur1 octave]$ cat func.txt
v = rand(10,1);

function average = avg (a)
  average = sum(a)/length(a) ;
endfunction

function [max,id] = vmax(a)
  id = 1;
  max = a(id);
  for i = 2:length(a)
    if ( a(i) > max )
      max = a(i) ;
      id = i ;
    endif
  endfor
endfunction

b = rand(20,1);
[max,id] = vmax(b);

printf ( ``Average of vector v = %f\n’’, avg(v))
printf ( ``Maximum value of vector b = %f with id = %d\n’’,max,id )

[apacheco@tezpur1 octave]$ octave -q
octave:1> source(’func.txt’)
Average of vector v = 0.487381
Maximum value of vector b = 0.878363 with id = 14
```

Script Files ***III***

- Octave also allows you to create an executable script file.
- The first line of the executable script file should refer the interpreter.
- Octave Executable scripts can take command line arguments.
- The built-in function `argv` returns a cell array containing the command line arguments passed to the executable script.
- The built-in function `nargin` returns the number of arguments passed.
- On Tezpur, first line should be

```
#!/usr/local/packages/octave/3.0.3/intel-11.1/bin/octave -qf
```

Script Files IV

```
[apacheco@tezpur1 octave]$ cat func.sh
#!/usr/local/packages/octave/3.0.3/intel-11.1/bin/octave -qf

v = rand(10,1);

function average = avg (a)
  average = sum(a)/length(a) ;
endfunction

function [max,id] = vmax(a)
  id = 1;
  max = a(id);
  for i = 2:length(a)
    if ( a(i) > max )
      max = a(i) ;
      id = i ;
    endif
  endfor
endfunction

b = rand(20,1);
[max,id] = vmax(b);

printf ( ``Average of vector v = %f\n'', avg(v))
printf ( ``Maximum value of vector b = %f with id = %d\n'',max,id )

[apacheco@tezpur1 octave]$ ls -l func.sh
-rwxr-xr-x  1 apacheco Admins 450 Apr 16 11:39 func.sh
```

Script Files V

```
[apacheco@tezpur1 octave]$ ./func.sh
Average of vector v = 0.599684
Maximum value of vector b = 0.986472 with id = 15
```

Calculate Spectra from AIMD Simulation I

- Octave script to calculate Fourier Transform of Auto-Correlation Function of Mass Weighted Velocities. /home/apacheco/octave-tutorial/getftmwvels.sh

```
[apacheco@tezpur1 octave-tutorial]$ cat getftmwvels.sh
#!/usr/local/packages/octave/3.0.3/intel-11.1/bin/octave -qf

if(nargin!=4)
   printf (``%s\n'', ``This script needs 4 arguments, [Velocity File (input)], \
        [FT-VAC File (output)], [Number of Atoms], [Time Step in fs]'' )
endif

arg_list = argv();
printf (``Argument list:'');
for i = 1:nargin
  printf (`` %s'', arg_list{i});
endfor
printf (``\n'');

Vels = arg_list{1};
VelsFT = arg_list{2};
NAtoms = eval(arg_list{3});
deltat = eval(arg_list{4});

M = NAtoms*3;
mwvels = load(Vels);
N = rows(mwvels);
ftmwvels = abs(fft(mwvels,N));
fid = fopen(VelsFT,''w'');
```

Calculate Spectra from AIMD Simulation II

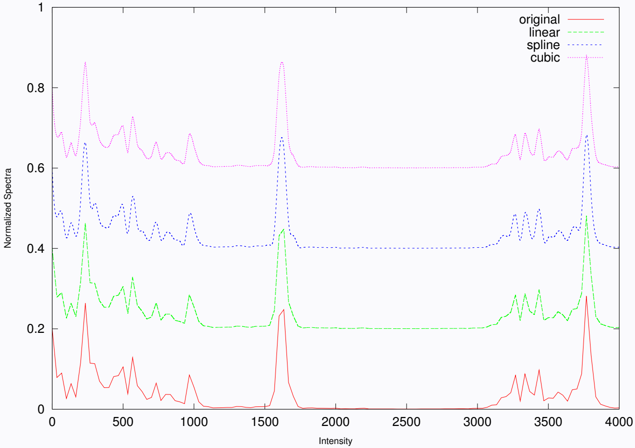
```
dw = 1/(N*deltat);
for I=[1:N]
  sumft=0;
  for J=[1:M]
    sumft=sumft+ftmwvels(I,J)^2;
  endfor
  fprintf(fid,’’ %15.8e  %21.14e\n’’,(I-1)*dw,sumft);
endfor
fclose(fid);

# Below was added for octave tutorial
A=load(VelsFT);
int=A(:,1)*33356; # convert from fs^-1 to cm^-1
spectra_orig=A(:,2)/norm(A(:,2)); # normalized original spectra
# Do interpolation of Spectra for octave demo
intensity=linspace(0,4000,400000);
# Linear Interpolation
spectra_lin=interp1(int,spectra_orig,intensity,’linear’);
# Spline Interpolation
spectra_spl=interp1(int,spectra_orig,intensity,’spline’);
# Cubic Interpolation
spectra_cub=interp1(int,spectra_orig,intensity,’cubic’);

plot(int,spectra_orig,’r’,intensity,spectra_lin+0.2,’g’, \
  intensity,spectra_spl+0.4,’b’,intensity,spectra_cub+0.6,’m’);

legend("original","linear","spline","cubic");
axis([0,4000,0,1]);
```

```
xlabel('Intensity');
ylabel('Normalized Spectra');

print -deps spectra.eps;
```

- Usage:

```
[apacheco@tezpur1 water-hexamer]$ ./getftmwvels.sh water-hexamer-cage-admp.mwvels \
> water-hexamer-cage-admp.ftmwvels 18 0.25
Argument list: water-hexamer-cage-admp.mwvels water-hexamer-cage-admp.ftmwvels 18 0.25

[apacheco@tezpur1 water-hexamer]$
```

Calculate Spectra from AIMD Simulation IV



References

1. Octave Manual: http://www.gnu.org/software/octave/doc/interpreter/index.html and http://www.gnu.org/software/octave/octave.pdf
2. Octave-Forge: http://octave.sourceforge.net/
3. Octave Tutorials: http://en.wikibooks.org/wiki/Octave_Programming_Tutorial