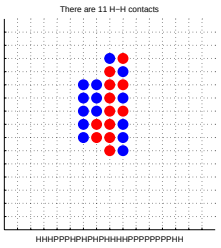
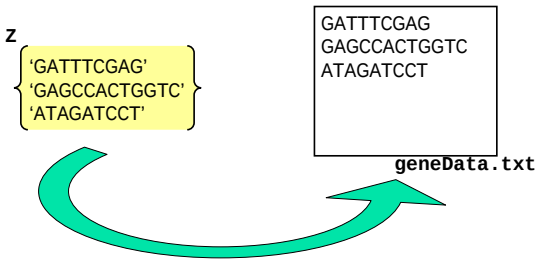
- Previous Lecture:
  - Structure
  - Structure arrays
- Today's Lecture:
  - Working with large data files
  - Built-in **`sort`** function
- Announcement:
  - P5 Part A posted, due 4/10 at 6pm
  - Part B TBA

Protein folding (Project 5)

- A protein is a sequence of amino acids
- Categorize amino acids as Hydrophobic and Polar
- "Fold" or layout amino acids to "hide" H's from the water



Example: Write a cell array of gene sequences to a file



A 3-step process to read data from a file or write data to a file

1. (Create and) open a file
2. Read data from or write data to the file
3. Close the file

1. Open a file

```
fid = fopen('geneData.txt', 'w');
```

An open file has a file ID, here stored in variable **`fid`**

Name of the file (created and) opened. **`txt`** and **`dat`** are common file name extensions for plain text files

Built-in function to open a file

'**`w`**' indicates that the file has been opened for **w**riting

2. Write (print) to the file

```
fid = fopen('geneData.txt', 'w');

for i=1:length(Z)
    fprintf(fid, '%s\n', Z{i});
end
```

Printing is to be done to the file with ID **`fid`**

Substitution sequence specifies the *string* format followed by a new-line character

The **`i`**th item in cell array **`Z`**

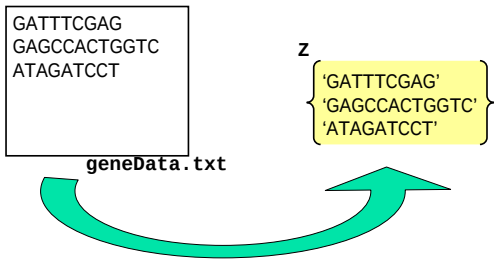
3. Close the file

```
fid = fopen('geneData.txt' ,'w');

for i=1:length(Z)
    fprintf(fid, '%s\n', Z{i});
end

fclose(fid);
```

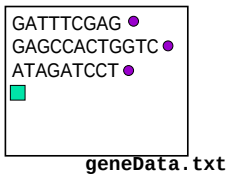


```
function cellArray2file(CA, fname)
% CA is a cell array of strings.
% Create a .txt file with the name
% specified by the string fname.
% The i-th line in the file is CA{i}

fid= fopen([fname '.txt'], 'w');
for i= 1:length(CA)
    fprintf(fid, '%s\n', CA{i});
end
fclose(fid);
```


Reverse problem: Read the data in a file line-by-line and store the results in a cell array



In a file there are hidden "markers"



- Carriage return marks the end of a line
- eof marks the end of a file

Read data from a file

1. Open a file
2. Read it line-by-line until eof
3. Close the file

1. Open the file

```
fid = fopen('geneData.txt', 'r');
```

- An open file has a file ID, here stored in variable **fid**
- Built-in function to open a file
- Name of the file opened. **txt** and **dat** are common file name extensions for plain text files
- '**r**' indicates that the file has been opened for reading

2. Read each line and store it in cell array

```
fid = fopen('geneData.txt', 'r');

k= 0;
while ~feof(fid)
   k= k+1;
   Z{k}= fgetl(fid);
end
```

False until end-of-file is reached

Get the next line

3. Close the file

```
fid = fopen('geneData.txt', 'r');

k= 0;
while ~feof(fid)
   k= k+1;
   Z{k}= fgetl(fid);
end
fclose(fid);
```



```
function CA = file2cellArray(fname)
% fname is a string that names a .txt file
%   in the current directory.
% CA is a cell array with CA{k} being the
%   k-th line in the file.

fid= fopen([fname '.txt'], 'r');
k= 0;
while ~feof(fid)
   k= k+1;
   CA{k}= fgetl(fid);
end
fclose(fid);
```


A Detailed Read-File Example

From the protein database at

http://www.rcsb.org

we download the file **1bl8.dat** which encodes the amino acid information for the protein with the same name. We want the xyz coordinates of the protein's "backbone".

The file has a long "header"

```
HEADER    MEMBRANE PROTEIN                        23-JUL-98   1BL8
TITLE     POTASSIUM CHANNEL (KCSA) FROM STREPTOMYCES LIVIDANS
COMPND    MOL_ID: 1;
COMPND   2 MOLECULE: POTASSIUM CHANNEL PROTEIN;
COMPND   3 CHAIN: A, B, C, D;
COMPND   4 ENGINEERED: YES;
COMPND   5 MUTATION: YES
SOURCE    MOL_ID: 1;
SOURCE   2 ORGANISM_SCIENTIFIC: STREPTOMYCES LIVIDANS;
```

Hundreds of lines—not relevant to us.

Eventually, the xyz data is reached…

```
MTRIX1   2 -0.736910 -0.010340  0.675910      112.17546    1
MTRIX2   2  0.004580 -0.999940 -0.010300       53.01701    1
MTRIX3   2  0.675980 -0.004490  0.736910      -43.35083    1
MTRIX1   3  0.137220 -0.931030  0.338160       80.28391    1
MTRIX2   3  0.929330  0.002860 -0.369240      -33.25713    1
MTRIX3   3  0.342800  0.364930  0.865630      -31.77395    1

ATOM      1  N   ALA A  23      65.191  22.037  48.576  1.00181.62       N
ATOM      2  CA  ALA A  23      66.434  22.838  48.377  1.00181.62       C
ATOM      3  C   ALA A  23      66.148  24.075  47.534  1.00181.62       C
```

x y z

Signal:Lines that begin with 'ATOM'

Where exactly are the xyz data?

```
1-4   14-15 18-20    33-38 41-46 49-54
```

Column nos. of interest

```
ATOM     14  N   HIS A  25      68.656  24.973  44.142  1.00128.26          N
ATOM     15  CA  HIS A  25      69.416  24.678  42.939  1.00128.26          C
ATOM     16  C   HIS A  25      68.843  23.458  42.227  1.00128.26          C
ATOM     17  O   HIS A  25      68.911  23.354  41.007  1.00128.26          O
ATOM     18  CB  HIS A  25      70.881  24.416  43.300  1.00154.92          C
ATOM     19  CG  HIS A  25      71.188  22.977  43.573  1.00154.92          C
ATOM     20  ND1 HIS A  25      71.886  22.184  42.689  1.00154.92          N
ATOM     21  CD2 HIS A  25      70.877  22.182  44.625  1.00154.92          C
ATOM     22  CE1 HIS A  25      71.993  20.963  43.183  1.00154.92          C
ATOM     23  NE2 HIS A  25      71.388  20.935  44.356  1.00154.92          N
ATOM     24  N   TRP A  26      68.271  22.546  43.005  1.00 87.09          N
ATOM     25  CA  TRP A  26      67.702  21.311  42.475  1.00 87.09          C
ATOM     26  C   TRP A  26      66.187  21.378  42.339  1.00 87.09          C
ATOM     27  O   TRP A  26      65.577  20.508  41.718  1.00 87.09          O
```

x y z

Just getting what you need from a data file

- Read past all the header information
- When you come to the lines of interest, collect the xyz data
  - Line starts with '**ATOM**'
  - Cols 18-19 is '**CA**'


```
fid = fopen('1bl8.dat','r');
x=[];y=[];z=[];
while ~feof(fid)
   s = fgetl(fid);
   if strcmp(s(1:4),'ATOM')
       if strcmp(s(18:19),'CA')
         x = [x; str2double(s(33:38))];
         y = [y; str2double(s(41:46))];
         z = [z; str2double(s(49:54))];
       end
   end
end
fclose(fid);
```

Open the file.


```
fid = fopen('1bl8.dat']);
x=[];y=[];z=[];
while ~feof(fid)
   s = fgetl(fid);
   if strcmp(s(1:4),'ATOM')
       if strcmp(s(18:19),'CA')
         x = [x; str2double(s(33:38))];
         y = [y; str2double(s(41:46))];
         z = [z; str2double(s(49:54))];
       end
   end
end
fclose(fid);
```

Initialize xyz arrays


```
fid = fopen('1bl8.dat']);
x=[];y=[];z=[];
while ~feof(fid)
   s = fgetl(fid);
   if strcmp(s(1:4),'ATOM')
       if strcmp(s(18:19),'CA')
         x = [x; str2double(s(33:38))];
         y = [y; str2double(s(41:46))];
         z = [z; str2double(s(49:54))];
       end
   end
end
fclose(fid);
```

Iterate Until End of File


```
fid = fopen('1bl8.dat']);
x=[];y=[];z=[];
while ~feof(fid)
   s = fgetl(fid);
   if strcmp(s(1:4),'ATOM')
       if strcmp(s(18:19),'CA')
         x = [x; str2double(s(33:38))];
         y = [y; str2double(s(41:46))];
         z = [z; str2double(s(49:54))];
       end
   end
end
fclose(fid);
```

Get the next line from file.

```
fid = fopen('1bl8.dat']);
x=[];y=[];z=[];
while ~feof(fid)
   s = fgetl(fid);
   if strcmp(s(1:4),'ATOM')
       if strcmp(s(18:19),'CA')
         x = [x; str2double(s(33:38))];
         y = [y; str2double(s(41:46))];
         z = [z; str2double(s(49:54))];
       end
   end
end
fclose(fid);
```

Make Sure It's a Backbone Amino Acid


```
fid = fopen('1bl8.dat']);
x=[];y=[];z=[];
while ~feof(fid)
   s = fgetl(fid);
   if strcmp(s(1:4),'ATOM')
       if strcmp(s(18:19),'CA')
         x = [x; str2double(s(33:38))];
         y = [y; str2double(s(41:46))];
         z = [z; str2double(s(49:54))];
       end
   end
end
fclose(fid);
```

Update the x, y, z arrays

Storing a numeric 2D array in a file

Have an array, e.g.,

```
>> A = rand(3,4)
A =
0.9218    0.4057    0.4103    0.3529
0.7382    0.9355    0.8936    0.8132
0.1763    0.9169    0.0579    0.0099
```


Storing a 2D array in a file

```
0.9218    0.4057    0.4103    0.3529
0.7382    0.9355    0.8936    0.8132
0.1763    0.9169    0.0579    0.0099
```

myMatrix.dat

Would like to specify the format, e.g., use **`%10.4f`** for each number.

Reason: Make it easier to read the file

`sprintf` returns a string

Example:

```
s = sprintf('h = %5d, x = %5.2f',h,x);
```


`sprintf` returns a string

Suppose **`x`** is a length-2 array. Then

```
s = sprint('%10.2f%10.2f',x(1),x(2))
```

is equivalent to

```
s = sprintf('%10.2f',x)
```

`sprintf` returns a string

Suppose `x` is a length-n array. Then

```
s = sprint('%10.2f',x);
```

is eqiuvalent to

```
s = [];
for i=1:length(x)
   s = [s sprintf('%10.2f',x(i))];
end
```


Storing a 2D array in a file

```
01234567890123456789012345678901234567890123456789
```

```
0.9218    0.4057    0.4103    0.3529
0.7382    0.9355    0.8936    0.8132
0.1763    0.9169    0.0579    0.0099
```

myMatrix.dat

```
fid = fopen('myMatrix.dat','w');
for i=1:3
   str = sprintf('%10.4f',M(i,:));
   fprintf(fid,'%s\n',str);
end
fclose(fid);
```

2D numeric array M → file

```
01234567890123456789012345678901234567890123456789
```

```
0.92      0.40      0.41      0.35
0.73      0.93      0.89      0.81
0.17      0.91      0.05      0.00
```

myMatrix.dat

```
fid = fopen('myMatrix.dat','w');
for i=1:3
   str = sprintf('%10.2f',M(i,:));
   fprintf(fid,'%s\n',str);
end
fclose(fid);
```

2D Numeric Array → File

```
01234567890123456789012345678901234567890123456789
```

```
0.921829 0.405785 0.410653 0.352999
0.738214 0.935564 0.893678 0.813275
0.176322 0.916909 0.057998 0.009957
```

myMatrix.dat

```
fid = fopen('myMatrix.dat','w');
for i=1:3
   str = sprintf('%9.6f',M(i,:));
   fprintf(fid,'%s\n',str);
end
fclose(fid);
```

```
function matrix2file(M,nbrFormat,fname)
% M is a 2D array of numbers
% Creates .dat file with name specified by the
%   string fname.
% The ith line in the file is M(i,:) displayed with
%   the format specified by the string nbrFormat

[nr,nc] = size(M);
fid = fopen([fname '.dat'],'w');
for i=1:nr
     str = sprintf(nbrFormat,M(i,:));
     fprintf(fid,'%s\n',str);
end
fclose(fid);
```


Try these examples

Suppose M is a real 2D array:

```
matrix2File(M,'%10d','MyMat')
matrix2File(M,'%9.2f','MyMat')
matrix2File(M,'%10.3e','MyMat')
```

A detailed sort-a-file example

Suppose each line in the file

statePop.txt

is structured as follows:

Cols 1-14: State name
Cols 16-24: Population (millions)

The states appear in alphabetical order.


```
Alabama          4557808
Alaska            663661
Arizona          5939292
Arkansas         2779154
California      36132147
Colorado         4665177
   :                :
   :                :
Texas           22859968
Utah             2469585
Vermont           623050
Virginia         7567465
Washington       6287759
West Virginia    1816856
Wisconsin        5536201
Wyoming           509294
```


A detailed sort-a-file example

Create a new file

statePopSm2Lg.txt

that is structured the same as **statePop.txt** except that *the states are ordered from smallest to largest according to population.*

First, get the populations into an array

```
C = file2cellArray('StatePop');
n = length(C);
pop = zeros(n,1);
for i=1:n
  S = C{i};
  pop(i) = str2double(S(16:24));
end
```


Built-In function **sort**

Syntax: `[y,idx] = sort(x)`

x:	10	20	5	90	15
y:	5	10	15	20	90
idx:	3	1	5	2	4

`y(1) = x(3) = x(idx(1))`

Built-In function **sort**

Syntax: `[y,idx] = sort(x)`

x:	10	20	5	90	15
y:	5	10	15	20	90
idx:	3	1	5	2	4

`y(2) = x(1) = x(idx(2))`

Built-In function **sort**

Syntax: **[y,idx] = sort(x)**

X:	10	20	5	90	15
y:	5	10	15	20	90
idx:	3	1	5	2	4

y(3) = x(5) = x(idx(3))

Built-In function **sort**

Syntax: **[y,idx] = sort(x)**

X:	10	20	5	90	15
y:	5	10	15	20	90
idx:	3	1	5	2	4

y(4) = x(2) = x(idx(4))

Built-In function **sort**

Syntax: **[y,idx] = sort(x)**

X:	10	20	5	90	15
y:	5	10	15	20	90
idx:	3	1	5	2	4

y(5) = x(4) = x(idx(5))

Built-In function **sort**

Syntax: **[y,idx] = sort(x)**

X:	10	20	5	90	15
y:	5	10	15	20	90
idx:	3	1	5	2	4

y(k) = x(idx(k))

Sort from little to big

```
% C is cell array read from statePop.txt
% pop is vector of state pop (numbers)
[s,rank] = sort(pop);
Cnew = cell(n,1);
for i=1:length(C)
    ithSmallest = rank(i);
    Cnew{i} = C{ithSmallest};
end

cellArray2file(Cnew,'statePopSm2Lg')
```



```
Wyoming          509294
Vermont          623050
North Dakota     636677
Alaska           663661
South Dakota     775933
Delaware         843524
Montana          935670
   :                :
   :                :
Illinois       12763371
Florida        17789864
New York       19254630
Texas          22859968
California     36132147
```