Parallel MATLAB jobs on Biowulf

Dave Godlove, HPC @ NIH
david.godlove@nih.gov

February 17, 2016

While waiting for the class to begin, log onto Helix and execute the following command

```
$ cp –r /data/classes/matlab/swarm_example /data/$USER
```

Outline

- Steps to running parallel MATLAB jobs
  - Developing code interactively
  - Compiling code
  - Writing swarm files and calling swarm
  - Monitoring jobs
- A concrete example (processing image files)

```
$ cp –r /data/classes/matlab/swarm_example /data/$USER
```

Quick review of a few MATLAB tricks

`fprintf`

```
>> name='Mary'; adjective='little'; noun='lamb'

>> fprintf('%s had a %s %s. \n',name,adjective,noun)

Mary had a little lamb.
>>
```

Quick review of a few MATLAB tricks

`sprintf`

```
>> name='Mary'; adjective='little'; noun='lamb'

>> sentence = ...
      sprintf('%s had a %s %s. \n',name,adjective,noun);

>> sentence

sentence =

Mary had a little lamb.
```

Quick review of a few MATLAB tricks

`eval`

```
>> part1='6'; part2='7';

>> eval(['ultimate_answer = ' part1 ' * ' part2])

ultimate_answer =

      42
```

Quick review of a few MATLAB tricks

```
eval(sprintf('command'))
```

```
>> part1='6'; part2='7';

>> eval(sprintf('ultimate_answer = %s * %s',part1,part2))

ultimate_answer =

      42
```

Quick review of a few MATLAB tricks

evalc

```
>> part1='6'; part2='7';

>> my_string = ...
       evalc(sprintf('ultimate_answer = %s * %s',part1,part2));

>> my_string

my_string =

ultimate_answer =

       42
```

Quick review of a few MATLAB tricks

! (pronounced bang, similar to system)

```
>> whoami
Undefined function or variable 'whoami'.

>> !whoami
godlovedc

>> user = evalc('!whoami'), host = evalc('!hostname')

user =
godlovedc

host =
cn1653
```

Quick review of a few MATLAB tricks

`fprintf`

`sprintf`

`eval`

`evalc`

`!`

Outline

- Steps to running parallel MATLAB jobs
  - Developing code interactively
  - Compiling code
  - Writing swarm files and calling swarm
  - Monitoring jobs
- A concrete example (processing image files)

```
$ cp –r /data/classes/matlab/swarm_example /data/$USER
```

Outline

- Steps to running parallel MATLAB jobs
  - Developing code interactively
  - Compiling code
  - Writing swarm files and calling swarm
  - Monitoring jobs
- A concrete example (processing image files)

```
$ cp –r /data/classes/matlab/swarm_example /data/$USER
```

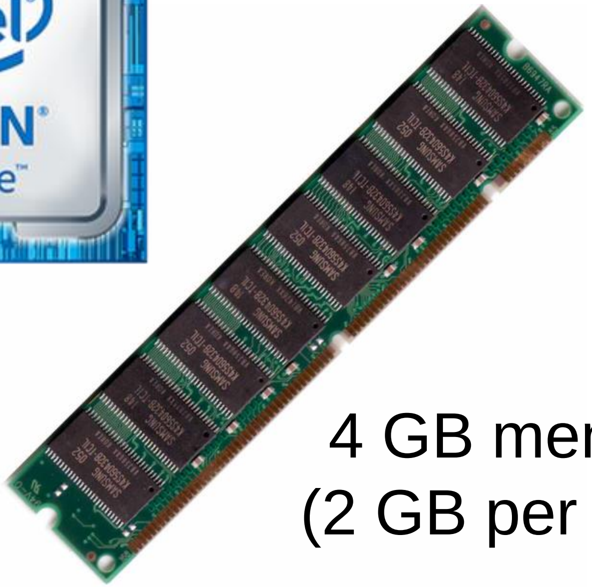
Quick overview of the cluster

Biowulf login node

Quick overview of the cluster

Biowulf login node

2 CPUs
(1 hyperthreaded core)



4 GB memory
(2 GB per CPU)

Quick overview of the cluster

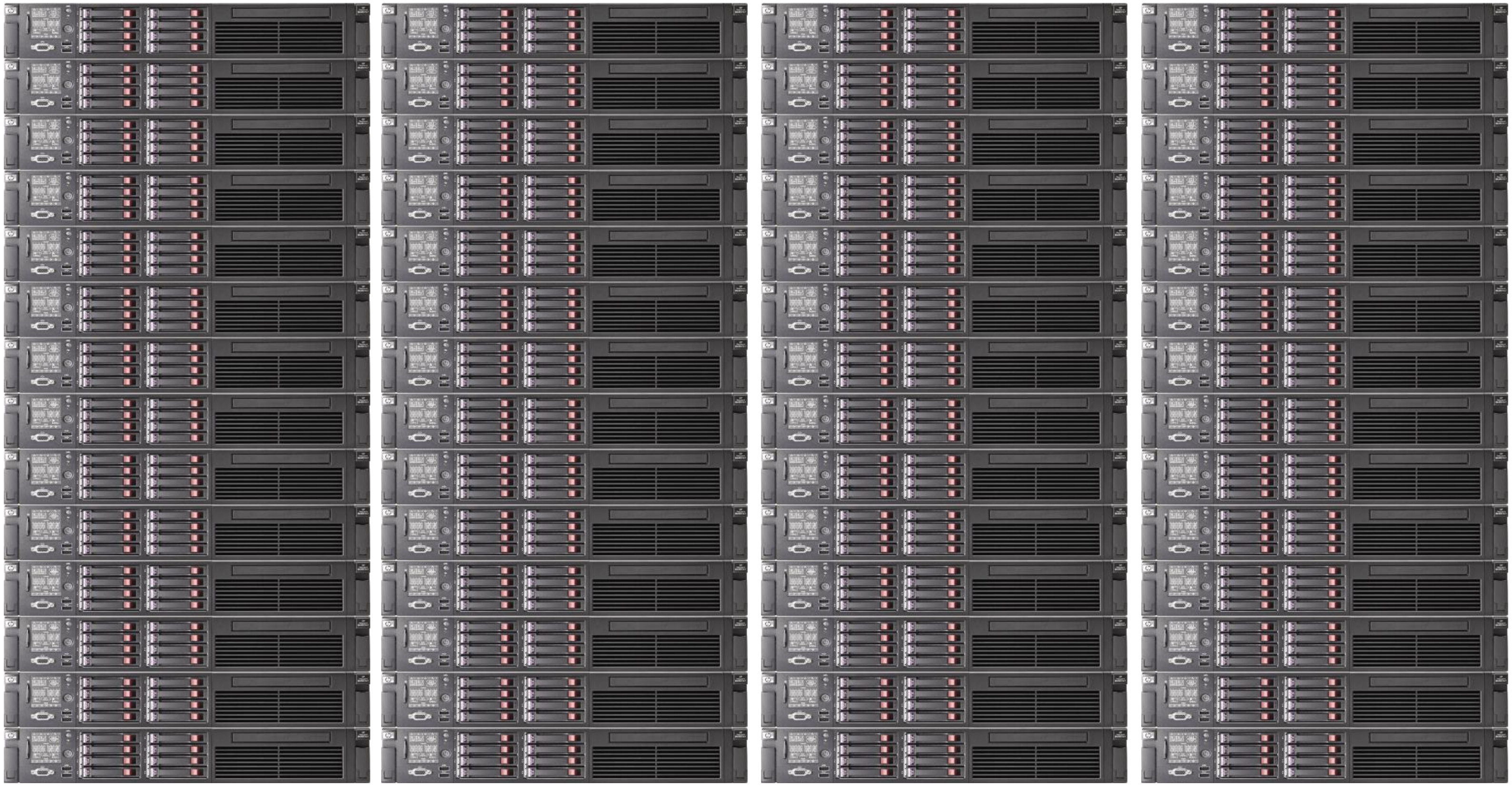
Biowulf login node

Biowulf compute node

Quick overview of the cluster

Biowulf login node

Biowulf partition

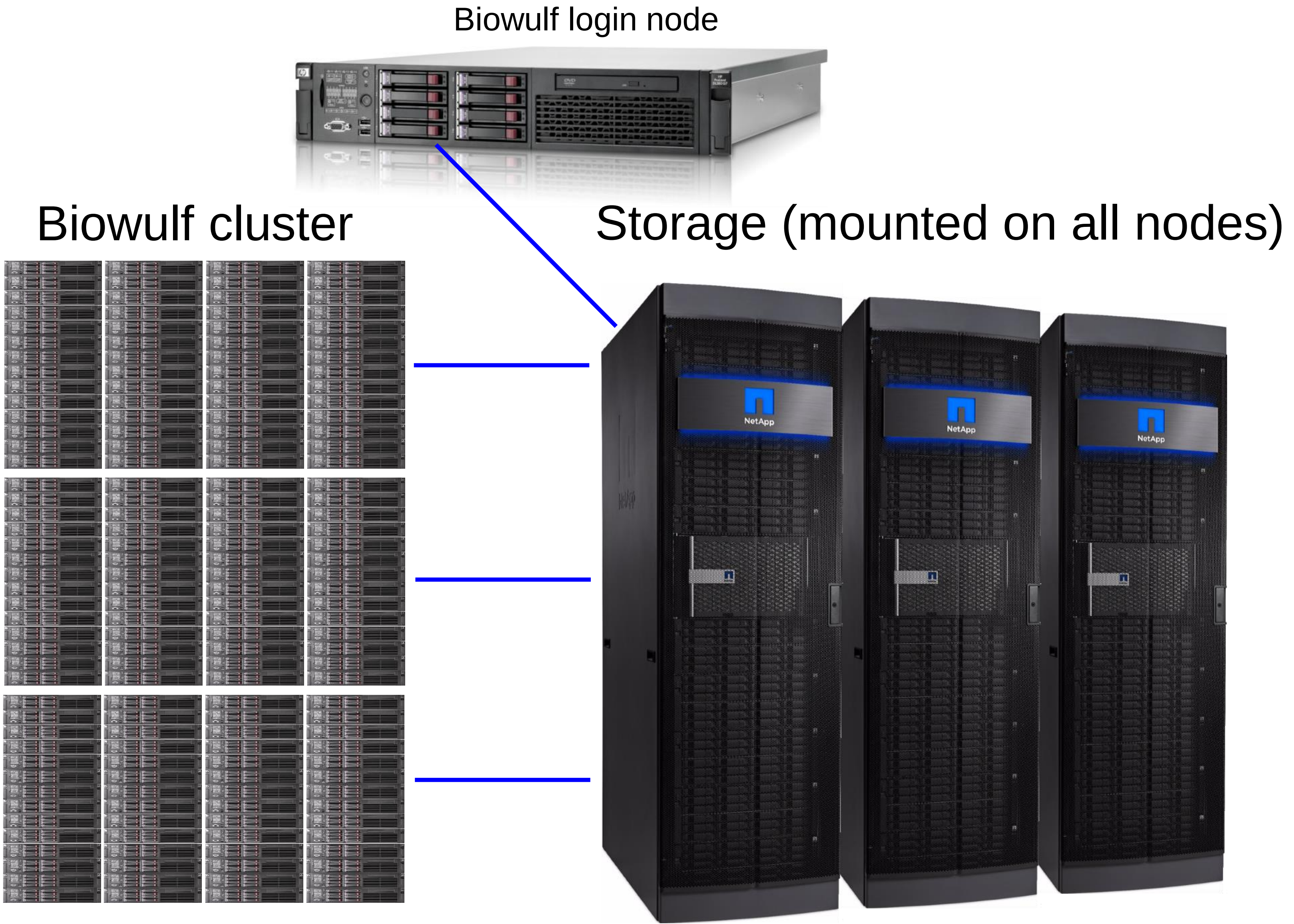


Quick overview of the cluster

Biowulf login node

Biowulf cluster

Quick overview of the cluster



Biowulf login node

Biowulf cluster

Storage (mounted on all nodes)

Developing code interactively

The steps to starting an interactive MATLAB session on a Biowulf compute node

```
$ ssh -Y user@biowulf.nih.gov

$ sinteractive -c 4 --mem=4g -L matlab,matlab-image,matlab-stat,matlab-compiler

$ module load matlab/<ver>
```

Two options, GUI or command prompt

```
$ matlab&
```

Or

```
$ matlab -nojvm
```

Developing code interactively

Using ssh to start a secure shell session on biowulf

```
$ ssh -Y user@biowulf.nih.gov
```

This step my differ depending on the client

- putty
- X-Win32
- XQuartz
- NoMachine (preferred client / available for Windows, Mac and Linux,)

https://hpc.nih.gov/docs/connect.html

Developing code interactively

Using sinteractive to allocate resources

```
$ sinteractive -c 4 --mem=4g -L matlab,matlab-image,matlab-stat,matlab-compiler
```

Developing code interactively

Loading modules

```
$ module load matlab
```

Or

```
$ module load matlab/2015b
```

```
$ module load matlab/2014b
```

etc...

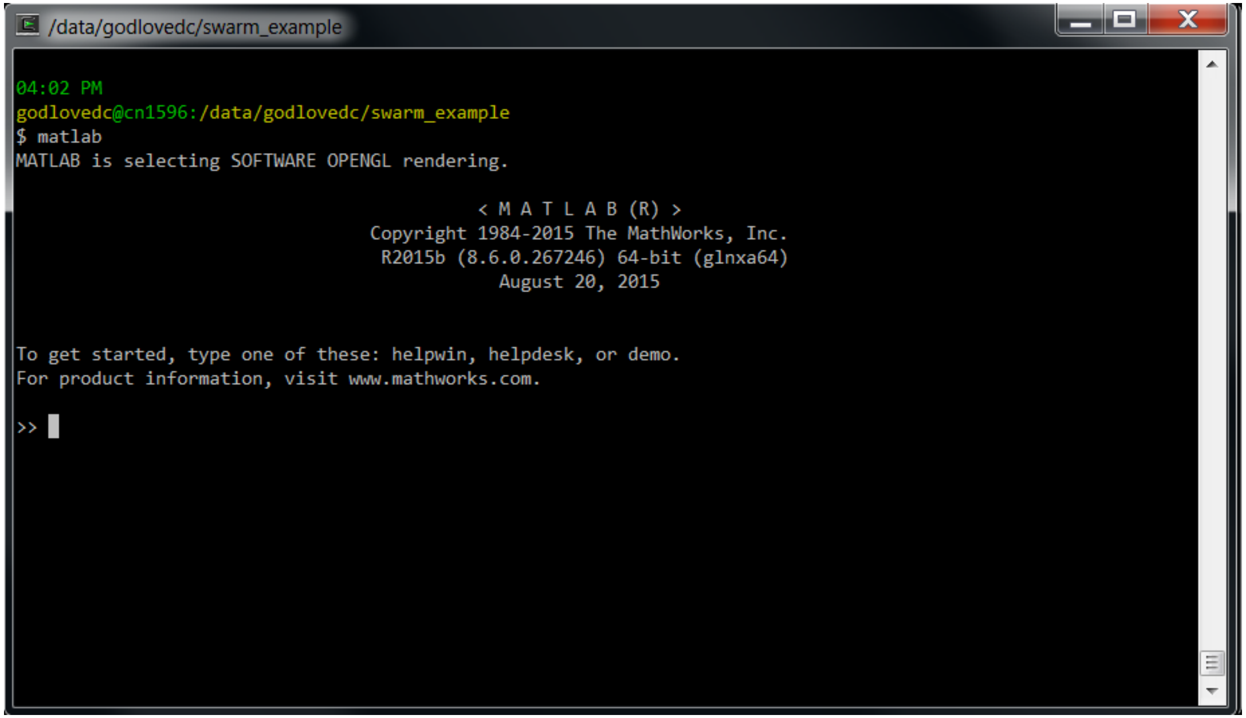
Developing code interactively

GUI vs. command line MATLAB

```
$ matlab&
```

Or

```
$ matlab -nojvm
```



```
04:02 PM
godlovedc@cn1596:/data/godlovedc/swarm_example
$ matlab
MATLAB is selecting SOFTWARE OPENGL rendering.

                                            < M A T L A B (R) >
                                  Copyright 1984-2015 The MathWorks, Inc.
                                   R2015b (8.6.0.267246) 64-bit (glnxa64)
                                              August 20, 2015


To get started, type one of these: helpwin, helpdesk, or demo.
For product information, visit www.mathworks.com.

>> 
```

Outline

- Steps to running parallel MATLAB jobs
  - Developing code interactively
  - Compiling code
  - Writing swarm files and calling swarm
  - Monitoring jobs
- A concrete example (processing image files)

```
$ cp –r /data/classes/matlab/swarm_example /data/$USER
```

Outline

- Steps to running parallel MATLAB jobs
    - Developing code interactively
    - Compiling code
    - Writing swarm files and calling swarm
    - Monitoring jobs
- A concrete example (processing image files)

```
$ cp –r /data/classes/matlab/swarm_example /data/$USER
```

Compiling code

Overview

- Removes the need for MATLAB licenses
- Allows you to run hundreds or thousands of instances of your code in parallel

Compiling code

Overview

Using a command like the following:

```
$ mcc2 –m my_function.m
```

or

```
>> mcc2 -m my_function.m
```

or

```
>> mcc2('-m','my_function.m')
```

Compiling code

Overview

produces several new files
(from my_function.m)

my_function	binary
run_my_function.sh	shell wrapper used to invoke my_function
readme.txt	some useful info (version of MATLAB)
mccExcludedFiles.log	lists some files that cannot be compiled
requiredMCRProducts.txt	not human readable?

Compiling code

Overview

Execute compiled code using the shell script:

```
$ run_my_function.sh /usr/local/matlab-compiler/v90 input1 input2 inputN
```

Compiling code

- Before you begin
  - Consider suppressing non-diagnostic output and figures
  - Will not be seen by user during execution and may complicate output (.o) files.

Compiling code

Before you begin

Can use the isdeployed flag:

```
% isdeployed evaluates to “true” if code is
% compiled here we say if not deployed plot a
% figure and pause
if ~isdeployed
   figure
   plot(x,y)
   pause
end
```

Compiling code

- Before you begin
  - Every function must be on your path at compile time.

Compiling code

Before you begin

Every function must be on your path **at compile time**!

No `addpath('/new/path')` statements!

Avoid `cd('/new/path')` statements too!

Compiling code

Before you begin

Compiled code will only accept strings as input

```
$ run_my_function.sh /usr/local/matlab-compiler/v90 input1 input2 inputN
```

For example:

```
$ run_my_function.sh /usr/local/matlab-compiler/v90 3 [1 2 5] {1,2,5}
```

Will be interpreted as:

```
>> my_function('3','[1 2 5]','{1,2,5}')
```

Compiling code

Before you begin

Code must convert strings back to their intended data types

```
input1 = char2double(input1);

eval(sprintf('input1 = %s;',input1))
```

Compiling code

Before you begin

Code must convert strings back to their intended data types

```
% this will check to see if the variable (var) is
% string and will convert it to strings value
if ischar(input1)
   eval(sprintf('input1 = %s;',input1))
end
```

Compiling code

When ready to compile, `mcc` is the proper command.

```
>> mcc -m my_function.m
```

But don't use it!

It will tie the compiler license up for as long as your MATLAB session is active!

Compiling code

Instead, use `mcc2` (wrapper to `mcc`)

```
>> mcc2 -m my_function.m
```

Opens a new instance of MATLAB, calls `mcc` to compile code, then closes new instance of MATLAB to release compiler license.

Available from MATLAB interactive sessions or from the shell (after loading MATLAB module).

Compiling code

Use the following command if `mcc2` does not appear on your search path.

```
>> rehash toolbox
```

Compiling code

Runtime flags

-singleCompThread
-nodisplay
-nojvm

For example:

```
>> mcc2 -m -R -nodisplay -R -singleCompThread my_function.m
```

Compiling code

Using the correct component runtime

```
$ run_my_function.sh /usr/local/matlab-compiler/v90 input1 input2 inputN
```

```
MATLAB version  runtime library
--------------  ---------------
         2015b              v90
         2015a              v85
         2014b              v84
         2013a              v81
         2012b              v80
```

More info at:
https://hpc.nih.gov/apps/Matlab_compiler.html

Compiling code

Using a local mcr cache

```
$ ls -al | grep mcr
drwxr-x---   10 godlovedc godlovedc      4096 Nov 10 11:04 .mcrCache8.0
drwxr-xr-x    6 godlovedc godlovedc     32768 Jan 27 10:51 .mcrCache8.1
drwxr-x---    5 godlovedc godlovedc     73728 Jan 27 11:25 .mcrCache8.4
drwxr-x---   13 godlovedc godlovedc      8192 Oct 28 12:06 .mcrCache8.5
drwxr-x---   14 godlovedc godlovedc     24576 Feb 16 01:28 .mcrCache9.0
```

Compiling code

Using a local mcr cache

```
$ export MCR_CACHE_ROOT=/tmp/$USER/mcr_cache

or

>> user = deblank(evalc('!whoami'));
>> setenv('MCR_CACHE_ROOT',fullfile('/tmp',user,'mcr_cache'))
```

Outline

- Steps to running parallel MATLAB jobs
  - Developing code interactively
  - Compiling code
  - Writing swarm files and calling swarm
  - Monitoring jobs
- A concrete example (processing image files)

```
$ cp –r /data/classes/matlab/swarm_example /data/$USER
```

Outline

- Steps to running parallel MATLAB jobs
  - Developing code interactively
  - Compiling code
  - Writing swarm files and calling swarm
  - Monitoring jobs
- A concrete example (processing image files)

```
$ cp –r /data/classes/matlab/swarm_example /data/$USER
```

Writing swarm files and calling swarm

- Swarm is a wrapper for sbatch
- Creates 1 job per line (in a job array)
- Greatly simplifies job submission
- Tons of options
- Can capture sbatch commands if useful

Writing swarm files and calling swarm

Overview: two step process

- Write a swarm file that has a single command (job) on each line
- Invoke the swarm program using the name of the swarm file as an argument

Writing swarm files and calling swarm

Example swarm file:
myjobs.swarm

```
run_my_function.sh /usr/local/matlab-compiler/v90 param1
run_my_function.sh /usr/local/matlab-compiler/v90 param2
run_my_function.sh /usr/local/matlab-compiler/v90 param3
run_my_function.sh /usr/local/matlab-compiler/v90 paramN

$ swarm -f myjobs.swarm
```

Writing swarm files and calling swarm

Generating swarm files in MATLAB

```
% stick all the parameters in an array
param_list = {'param1' 'param2' 'param3' 'paramN'};

% make a command on a new line for each parameter
command_list = [];
for ii = 1:length(param_list)
    command_list = [command_list ...
        'run_my_function.sh '...
        '/usr/local/matlab-compiler/v90 '...
        param_list{ii}...
        '\n'];
end

% write the commands into a swarm file
file_handle = fopen('myjobs.swarm','w+');
fprintf(file_handle,command_list);
fclose(file_handle);
```

Writing swarm files and calling swarm

Example swarm file:
myjobs.swarm

```
run_my_function.sh /usr/local/matlab-compiler/v90 param1
run_my_function.sh /usr/local/matlab-compiler/v90 param2
run_my_function.sh /usr/local/matlab-compiler/v90 param3
run_my_function.sh /usr/local/matlab-compiler/v90 paramN
```

Writing swarm files and calling swarm

Remember:
Inputs are strings

```
run_my_function.sh /usr/local/matlab-compiler/v90 1
run_my_function.sh /usr/local/matlab-compiler/v90 2
run_my_function.sh /usr/local/matlab-compiler/v90 3
run_my_function.sh /usr/local/matlab-compiler/v90 4
```

Writing swarm files and calling swarm

Arrays as input to compiled functions

```
param1 =

     4     1     0     2
     4     4     0     5
     2     0     4     0
     3     1     3     2

>> param1 = ['"' mat2str(param1) '"']

param1 =

"[4 1 0 2;4 4 0 5;2 0 4 0;3 1 3 2]"
```

Writing swarm files and calling swarm

Arrays as input to compiled functions

```
run_my_function.sh /usr/local/matlab-compiler/v90 "[4 1 0 2;4 4 0 5;2 0 4 0;3 1 3 2]"
run_my_function.sh /usr/local/matlab-compiler/v90 "[2 2 4 1;4 2 1 1;4 3 3 2;1 4 3 5]"
run_my_function.sh /usr/local/matlab-compiler/v90 "[2 1 5 1;3 3 3 4;1 3 1 1;4 4 1 4]"
…
run_my_function.sh /usr/local/matlab-compiler/v90 "[1 1 4 1;5 3 3 4;2 2 3 4;1 2 5 2]"
```

Writing swarm files and calling swarm

Arrays as input to compiled functions

```
param1 =

[4 1 0 2;4 4 0 5;2 0 4 0;3 1 3 2]

>> eval(sprintf('param1 = %s',param1))

param1 =

     4     1     0     2
     4     4     0     5
     2     0     4     0
     3     1     3     2
```

Writing swarm files and calling swarm

Cell arrays as input to compiled functions

```
>> param1 = {'Bill','Steve','Linus','Cleve'}

param1 =

    'Bill'    'Steve'    'Linus'    'Cleve'
```

Writing swarm files and calling swarm

Cell arrays as input to compiled functions

```
param1 = {'Bill','Steve','Linus','Cleve'}

param_str = [];
for ii = 1:length(param1)
    param_str = [param_str '''' param1{ii} '''' ','];
end

param1 = ['"{' param_str(1:end-1) '}"'];

>> param1

param1 =

"{'Bill','Steve','Linus','Cleve'}"
```

Writing swarm files and calling swarm

Cell arrays as input to compiled functions

```
run_my_function.sh /usr/local/matlab-compiler/v90 "{'Bill','Steve','Linus','Cleve'}"
run_my_function.sh /usr/local/matlab-compiler/v90 "{'Hank','Dean','Doc','Brock'}"
run_my_function.sh /usr/local/matlab-compiler/v90 "{'Sheila','Triana','Kim','Sally'}"
…
run_my_function.sh /usr/local/matlab-compiler/v90 "{'Walt','Jesse','Gus','Mike'}"
```

Writing swarm files and calling swarm

Cell arrays as input to compiled functions

```
param1 =

{'Bill','Steve','Linus','Cleve'}

>> eval(sprintf('param1 = %s',param1))

param1 =

    'Bill'    'Steve'    'Linus'    'Cleve'
```

Writing swarm files and calling swarm

.mat files as input

```
>> param = round(rand(4)*10)

param =

     4     1     0     2
     4     4     0     5
     2     0     4     0
     3     1     3     2
```

Writing swarm files and calling swarm

.mat files as input

```
% how many files?
fileN = 4;

% make a directory for .mat files
mat_dir = '~/mat_dir';
if ~isdir(mat_dir)
    mkdir(mat_dir)
end

% generate arrays and save in .mat files
for ii = 1:fileN
    param = round(rand(4)*10);
    filename = sprintf('%s.mat',num2str(ii));
    save(fullfile(mat_dir,filename),'param');
end
```

Writing swarm files and calling swarm

```
% list all the files in a directory
mat_dir = '~/mat_dir';
file_list = what(mat_dir);
file_list = file_list.mat;

% make a command on a new line for each file
command_list = [];
for ii = 1:length(file_list)
    command_list = [command_list ...
        'run_my_function.sh '...
        '/usr/local/matlab-comiler/v90 '...
        file_list{ii}...
        '\n'];
end

% write the commands into a swarm file
file_handle = fopen('myjobs.swarm','w+');
fprintf(file_handle,command_list);
fclose(file_handle);
```

Writing swarm files and calling swarm

.mat files as input

```
run_my_function.sh /usr/local/matlab-compiler/v90 1.mat
run_my_function.sh /usr/local/matlab-compiler/v90 2.mat
run_my_function.sh /usr/local/matlab-compiler/v90 3.mat
run_my_function.sh /usr/local/matlab-compiler/v90 4.mat
```

Writing swarm files and calling swarm

.mat files as input

```
function my_function(filename)

load(filename,'param')

% param =

  %   4     1     0     2
  %   4     4     0     5
  %   2     0     4     0
  %   3     1     3     2

% code that uses input1 below...
% ...
```

Writing swarm files and calling swarm

Calling swarm to run file in terminal

```
$ swarm -f myjobs.swarm
10258332
```

From within MATLAB

```
>> !swarm -f myjobs.swarm
10258333
```

Writing swarm files and calling swarm

Even better from within MATLAB (capture the job id)!

```
>> jobid = evalc('!swarm -f myjobs.swarm')

jobid =

10259035
```

Writing swarm files and calling swarm

Setting up dependencies with job ids

```
$ swarm -f myjobs.swarm
10258332

$ swarm -f anotherjob.swarm -dependency=afterany:10258332
```

Writing swarm files and calling swarm

Setting up dynamic dependencies with captured job ids in MATLAB

```
>> jobid = evalc('!swarm -f myjobs.swarm');

>> eval(sprintf('!swarm -f anotherjob.swarm dependency=afterany:%s',...
        jobid))

10258333
```

Writing swarm files and calling swarm

Setting up dynamic dependencies with captured job ids in MATLAB

```
>> jobid = evalc('!swarm -f job1.swarm');

>> jobid = evalc(sprintf('!swarm -f job2.swarm dependency=afterany:%s',...
      jobid));

>> jobid = evalc(sprintf('!swarm -f job3.swarm dependency=afterany:%s',...
      jobid));

>> jobid = evalc(sprintf('!swarm -f jobN.swarm dependency=afterany:%s',...
      jobid));
```

Etc…

Outline

- Steps to running parallel MATLAB jobs
  - Developing code interactively
  - Compiling code
  - Writing swarm files and calling swarm
  - Monitoring jobs
- A concrete example (processing image files)

```
$ cp –r /data/classes/matlab/swarm_example /data/$USER
```

Outline

- Steps to running parallel MATLAB jobs
  - Developing code interactively
  - Compiling code
  - Writing swarm files and calling swarm
  - Monitoring jobs
- A concrete example (processing image files)

```
$ cp –r /data/classes/matlab/swarm_example /data/$USER
```

Monitoring jobs

```
$ squeue -j 10258333
$ squeue -u username

$ jobload -j 10258333
$ jobload -u username

$ sjobs -j 10258333
$ sjobs -u username

$ jobhist jobid
```

Monitoring jobs dynamically

```
>> eval(sprintf('!squeue -j %s',jobid))
>> eval('!squeue $USER')

>> eval(sprintf('!jobload -j %s',jobid))
>> eval('!jobload $USER')

>> eval(sprintf('!sjobs -j %s',jobid))
>> eval('!sjobs $USER')

>> eval(sprintf('!jobhist %s',jobid))
```

Monitoring jobs

```
myjobs.o
myjobs.e
```

⌛ Time for a break