L16, 28 March: VisIt-HPC-batch

1) Launch these programs on your computer (lab or labtop)
FileZilla or Fugu
Putty or Terminal
NotePad++ or TextEdit or TextWrangler

2) With FileZilla or Fugu, connect to tezpur.hpc.lsu.edu and copy to your computer
Movie_MAS_2.py
visit_python_batch_script.txt

tezpur.hpc.lsu.edu port 22, path /project/lbutler

Open both up in NotePad++ or TextEdit or TextWrangler

Our to-do list:

1) Update a VisIt Python script. Edit a path so that calculated image files are stored in your tezpur directory.
2) Update a Philip batch script file so that it uses your VisIt Python script and emails to your account the job status information.

3) Create and verify your directory on tezpur in /project/lbutler/students

4) Update the .soft file in your account on Philip /home/your name
5) Create directory on Philip /home/your name/.visit/hosts/ and put a copy of host_philip.xml in this new directory.

6) Finally, submit a batch job.

Les Butler's experience with VisIt on HPC Philip

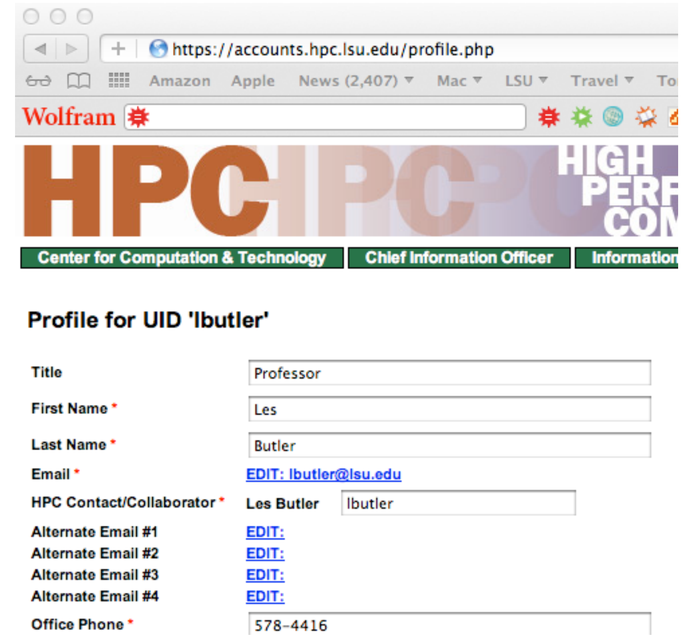
VisIt batch mode

(1) Is my account active? Yes

LSU

Account and Allocation Web Interface

- LONI: **allocations.loni.org**
- LSU HPC: **accounts.hpc.lsu.edu**
- This is where you
  - Request accounts
  - Request and manage allocations (for LONI only)
  - Update user profile
  - Reset password



Les is using bash shell

(2) Where is my terminal application?
It is in Macintosh /Applications/Utilities/Terminal.app

(3) Do I change from default preferences? No

I do use Terminal/View/Bigger to make the font bigger on large monitor system.

```
tomo3:wk11 tomo3$ pwd
/Volumes/Sab-Data-1/t4581/wk11
tomo3:wk11 tomo3$ ls -l
total 509656
-rw-------@  1 tomo3  staff    1323386 Mar 26 08:58 CHEM4581_HPC_Environment_20120326_draft.pdf
-rw-r--r--@  1 tomo3  staff     676441 Mar 28 09:03 L16_28Mar_VisIt-HPC-batch.key
-rw-r--r--   1 tomo3  staff     743668 Mar 28 08:49 L16_28Mar_VisIt-HPC-interactive.key
-rw-r--r--@  1 tomo3  staff    2075094 Mar 26 14:38 WindowsLogin.pdf
-rw-r--r--@  1 tomo3  staff      44709 Mar 26 15:50 emacs.pdf
-rw-r--r--   1 tomo3  staff  256001400 Mar 26 15:58 temp.h5
-rw-r--r--@  1 tomo3  staff      62661 Mar 26 15:47 vi_cheat sheet.pdf
drwxr-xr-x  10 tomo3  staff        340 Mar 27 17:38 visit_python
tomo3:wk11 tomo3$
```

VisIt batch mode

(4) Can I log in to Philip? Yes

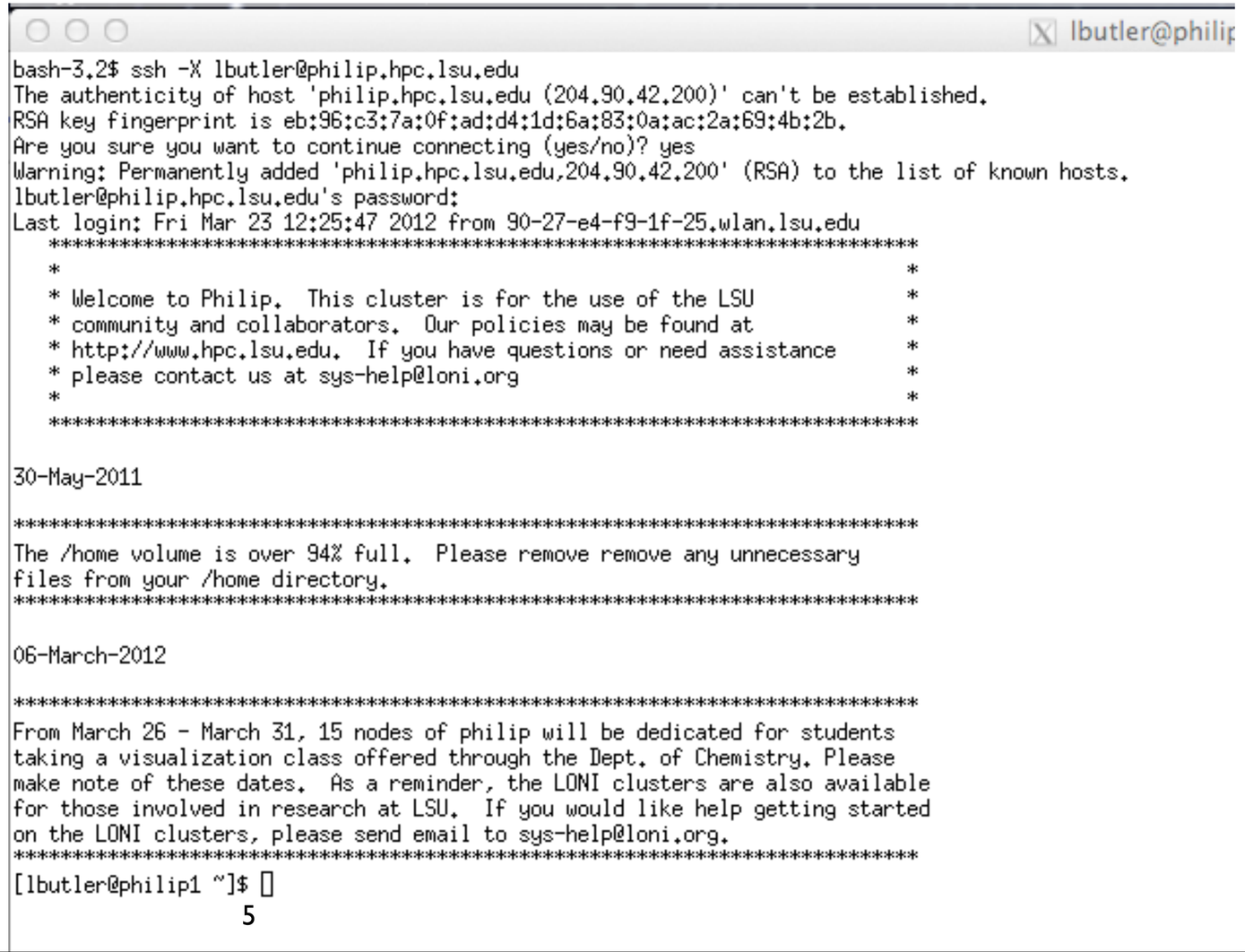
Turn on Terminal

At prompt, I typed ssh lbutler @philip.hpc.lsu.edu

For first time, I accepted philip as a “known host” by typing yes

Note: y or Y is not good enough.

This known host is part of the ssh security system.



(5) What are the contents of my home directory on Philip?

VisIt batch mode

Useful commands are:

ls list directory contents

ls -al list all contents (do not skip entries starting with .) and list the author of each file

```
[lbutler@philip1 ~]$ man ls
[lbutler@philip1 ~]$
[lbutler@philip1 ~]$
[lbutler@philip1 ~]$
[lbutler@philip1 ~]$ ls
[lbutler@philip1 ~]$
[lbutler@philip1 ~]$
[lbutler@philip1 ~]$ ls -al
total 104
drwx------   6 lbutler Users  4096 Mar 27 10:26 .
drwxr-xr-x 274 root    root  12288 Mar 26 12:42 ..
-rw-------   1 lbutler Users  3210 Mar 27 10:26 .bash_history
-rw-------   1 lbutler Users    95 Mar 26 16:38 .bash_history3
-rw-------   1 lbutler Users    33 Mar 23 12:15 .bash_logout
-rw-------   1 lbutler Users   176 Mar 23 12:15 .bash_profile
-rw-------   1 lbutler Users   124 Mar 23 12:15 .bashrc
-rw-------   1 lbutler Users   515 Mar 23 12:15 .emacs
drwx------   4 lbutler Users  4096 Mar 23 12:15 .mozilla
-rw-r--r--   1 lbutler Users   257 Mar 26 16:15 .soft
-rw-r--r--   1 lbutler Users 14557 Mar 26 16:16 .soft.cache.csh
-rw-r--r--   1 lbutler Users 15261 Mar 26 16:16 .soft.cache.sh
drwx------   2 lbutler Users  4096 Mar 23 12:15 .ssh
drwx------   2 lbutler Users  4096 Mar 23 12:15 .subversion
-rw-------   1 lbutler Users   611 Mar 26 16:15 .viminfo
drwxr-xr-x   4 lbutler Users  4096 Mar 26 16:36 .visit
-rw-------   1 lbutler Users   267 Mar 27 10:26 .Xauthority
-rw-------   1 lbutler Users   658 Mar 23 12:15 .zshrc
[lbutler@philip1 ~]$ Á
```

Not much in this home directory.

Well, a few hidden files. The important file is .soft

(6) What are the contents of the file .soft ?

Useful commands are:

more a file perusal filter for crt viewing

man access to help files for a command

VisIt batch mode

```
[lbutler@philip1 ~]$ man more
[lbutler@philip1 ~]$
[lbutler@philip1 ~]$ more .soft
#
# This is the .soft file.
# It is used to customize your environment by setting up environment
# variables such as PATH and MANPATH.
# To learn what can be in this file, use 'man softenv'.
#
+visit-2.3.2
+mpich2-1.4.1p1-gcc-4.3.2
+gcc-4.3.2
#
@default
[lbutler@philip1 ~]$
```

Just like Le Yan/Alex lecture, slides #20, #39

(7) BTW. At first login, .soft did not have the +visit-2.3.2 and other keys. I used the vi editor to enter keys for visit, mpich, and gcc into the .soft file. Alex has done the same for all students in this class.

(8) The instructions on slide #39 include.

VisIt batch mode

Useful commands are:

mkdir make directories
cd change directory
pwd print working directory (usually current directory).

- Copy the host profile to your home directory
  - cp /usr/local/packages/visit/host_philip.xml ~/.visit/hosts/

So, I typed (note: the dollar sign is the prompt character from Philip. I didn't type it).

$ mkdir .visit
$ cd .visit
$ pwd
and Philip printed /home/lbutler/.visit
$ mkdir hosts
$ cd hosts
$ pwd
and Philip printed /home/lbutler/.visit/hosts
$ cp /usr/local/packages/visit/host_philip.xml ~/.visit/hosts/
$ ls
and Philip printed host_philip.xml

(9) Do I have any data to visualize? *.h5 would be nice or *.bin, *.bov would be ok
The data is on tezpur which is accessible from Philip. Our class data is in /project/lbutler

VisIt batch mode

```
[lbutler@philip1 lbutler]$ cd /project/lbutler/
[lbutler@philip1 lbutler]$ ls -l
total 24
drwxr-sr-x  2 lbutler h3035 4096 Jan 12  2011 Avizo
drwxr-sr-x  6 zodhomb h3035 4096 Feb 18  2011 biology
drwxrwxrwx  6 kham    h3035 4096 Mar 16 09:03 camd
drwxr-sr-x  2 jinghua h3035 4096 Mar 12 15:06 class-data-spring12
drwxr-sr-x 11 lbutler h3035 4096 Jan 13  2011 data_materials
drwxr-sr-x  2 lbutler h3035 4096 Jan 28 14:43 hw3
```

I typed:
cd /project/lbutler
ls -l

```
[lbutler@philip1 lbutler]$ cd data_materials
[lbutler@philip1 data_materials]$ ls -l
total 36
drwxr-sr-x 2 lbutler h3035 4096 Mar 10 14:05 basalt
drwxr-sr-x 3 lbutler h3035 4096 Jan 21  2011 battery
drwxr-sr-x 2 lbutler h3035 4096 Jan 24  2011 bullet
drwxr-sr-x 3 lbutler h3035 4096 Feb 20  2011 hydrogen
drwxr-sr-x 2 lbutler h3035 4096 Mar 26 16:28 MAS_rotor
drwxr-sr-x 3 lbutler h3035 4096 Jan 25  2011 migmatite
drwxr-sr-x 2 lbutler h3035 4096 Feb  7 10:13 polymer_blend
drwxr-sr-x 3 lbutler h3035 4096 Jan 21  2011 polymer_constantheat
drwxr-sr-x 2 lbutler h3035 4096 Jan 26  2011 secret_stuff
[lbutler@philip1 data_materials]$ cd MAS_rotor/
[lbutler@philip1 MAS_rotor]$ ls -l
total 613524
-rw-r--r-- 1 lbutler h3035   8978571 Jan  7  2011 3035_MAS_rotor_Xray.mov
-rw-r--r-- 1 lbutler h3035   6173430 Jan 10  2011 3035_MAS_rotor_Xray.nb
-rw-r--r-- 1 lbutler h3035 435175000 Jan  7  2011 MAS-rotor_{650,650,515}_uint16.bin
-rw-r--r-- 1 lbutler h3035 177904292 Mar 26 16:28 MAS_rotor_cropped.h5
```

I typed:
cd data_ and then pressed tab
ls -l

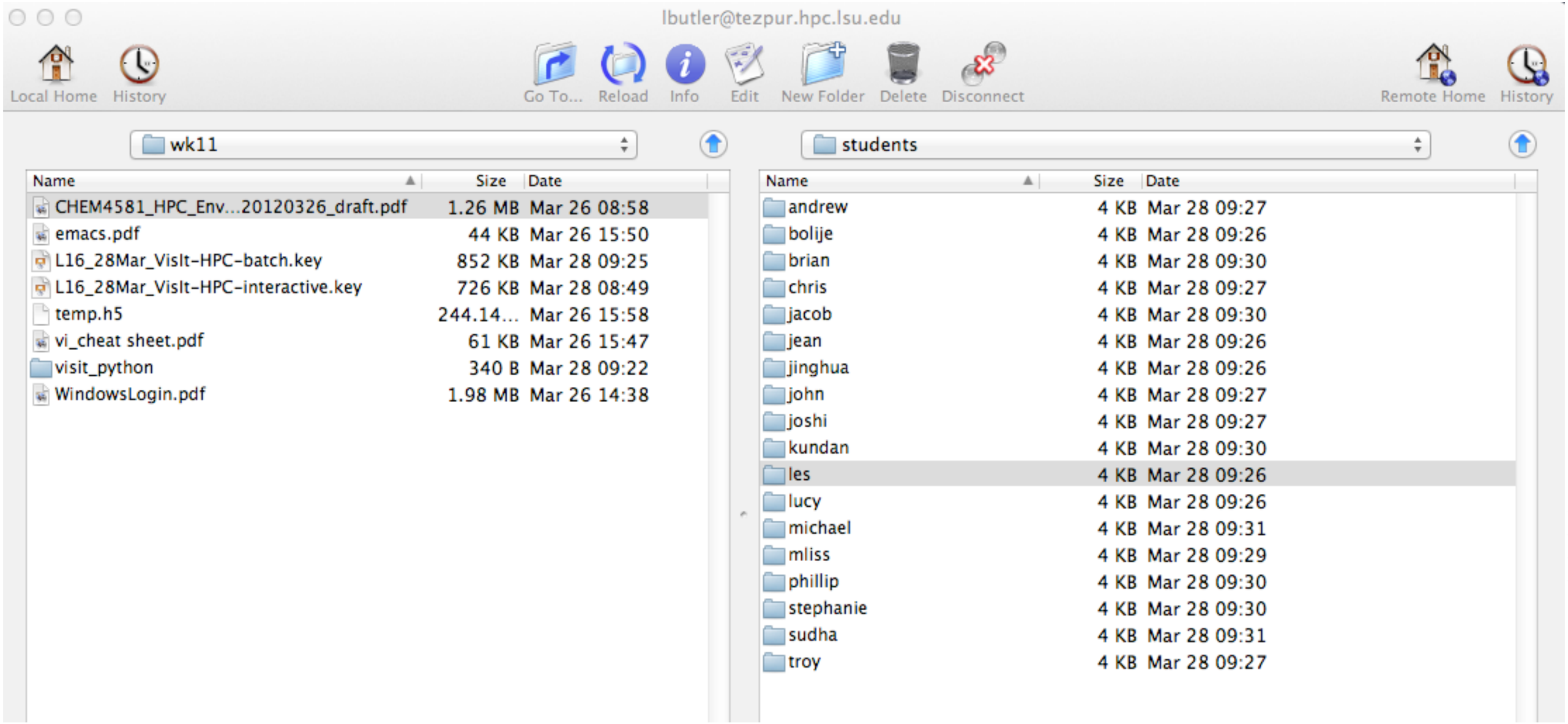
I typed:
cd MA and then pressed tab
ls -l

Found the data!!

(10) Where am I going to store my results?

VisIt batch mode

/project/lbutler/students/les



(11) Download from Moodle/Week 11/ two text files
Movie_MAS_2.py and visit_python_batch_script.txt

VisIt batch mode

Open visit_python_batch_script.txt in a text editor like NotePad+, TextWrangler, or similar

visit_python_batch_script.txt

Last Saved: 3/28/12 9:22:23 AM
File Path : /Volumes/Sab-Data-1/t4581/.../visit_python_batch_scri

visit_python_batch_script.txt

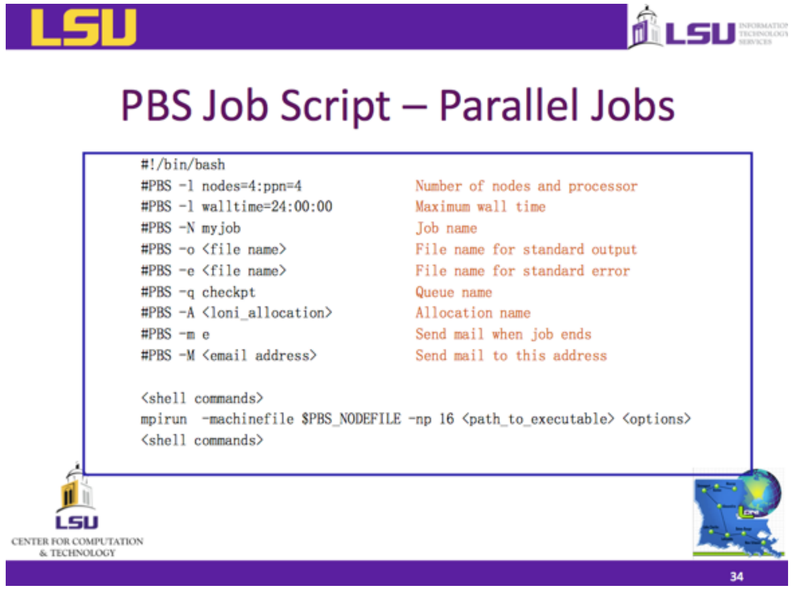
```
#!/bin/bash

#PBS -l nodes=4:ppn=8
#PBS -l walltime=00:30:00
#PBS -N visit_python
#PBS -o visit_python_output.txt
#PBS -e visit_python_error.txt
#PBS -q priority
#PBS -m e
#PBS -M lbutler@lsu.edu

cd ~
visit -cli -nowin -s /project/lbutler/students/les/Movie_MAS_2.py
```

Later, increase walltime as you gain experience with length of jobs.

Must change to your email.

Must change to your name.

This batch script file is taken from Le Yan's slide #34.



(12) Open Movie_MAS_2.py in a text editor

VisIt batch mode

Movie_MAS_2.py

Last Saved: 3/28/12 9:22:46 AM
File Path : /Volumes/Sab-Data-1/t4581/.../visit_python/Movie_MAS_2.py

Movie_MAS_2.py | (no symbol selected)

```
import os
import sys

# Read the *.h5 data file
OpenDatabase("/project/lbutler/data_materials/MAS_rotor/MAS_rotor_cropped.h5")

# Create window attributes.
s = SaveWindowAttributes()
s.format = s.JPEG
s.outputToCurrentDirectory = 0
s.outputDirectory = "/project/lbutler/students/les"
s.fileName = "Les_volume_increase_opacity_"
s.width, s.height = 600, 400
s.screenCapture = 0
s.progressive = 1
SetSaveWindowAttributes(s)

# Create a plot
AddPlot("Volume", "volMAS")
va = VolumeAttributes()
va.opacityAttenuation = 0.75
va.colorVarMin = 32500
va.useColorVarMin = 1
va.colorVarMax = 45000
va.useColorVarMax = 1
va.resampleTarget = 50000000
va.opacityMode = va.FreeformMode
```

This is good.

Must change to your name.
Both lines.

Note the really large value for samples.
This is a viz problem perfect for HPC.

(12) Continuing with Movie_MAS_2.py in a text editor

VisIt batch mode

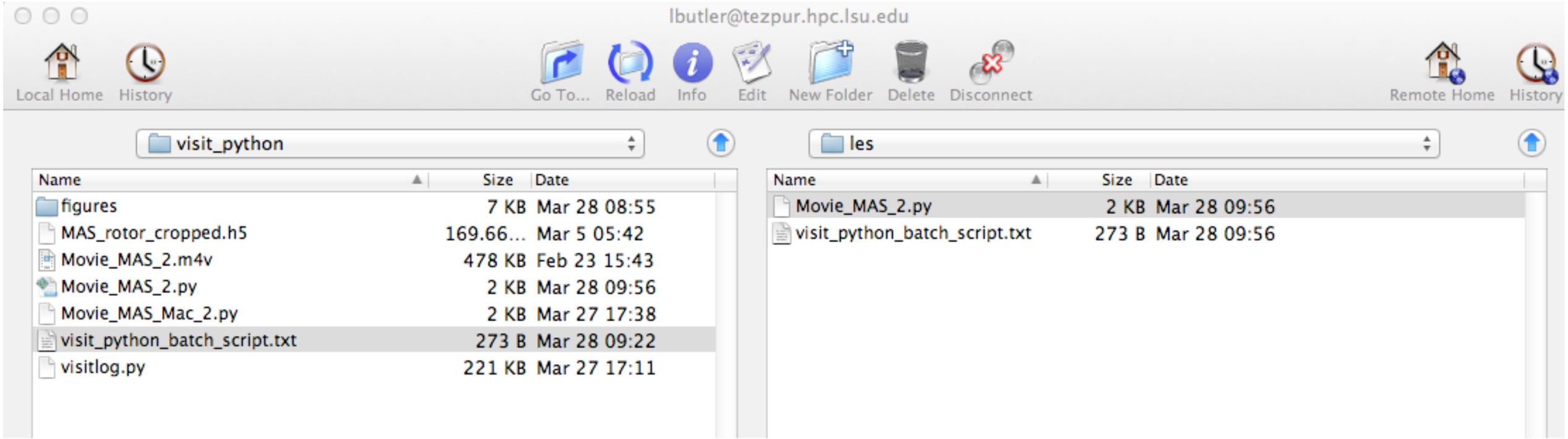
```
va.resampleTarget = 50000000
va.opacityMode = va.FreeformMode
SetPlotOptions(va)

# Draw the Plot
DrawPlots()

# Set the plot orientation
v0 = GetView3D()
v0.viewNormal = (0.80, 0.5, -0.50)
SetView3D(v0)
# print v0

# Turn off some of the labelling around the plot
legendLabelAxisStaff= AnnotationAttributes()
legendLabelAxisStaff.userInfoFlag = 0
legendLabelAxisStaff.databaseInfoFlag = 0
legendLabelAxisStaff.legendInfoFlag = 0
legendLabelAxisStaff.axes3D.visible = 0
legendLabelAxisStaff.axesArray.visible = 0
legendLabelAxisStaff.triadFlag = 0
SetAnnotationAttributes(legendLabelAxisStaff)

# Loop over a range of opacity values and save the plots
for j in range(255,5,-5):
    ffo = range(0,256)
    for i in ffo:
        if i <= j:
            ffo[i] = 0
        else:
            ffo[i] = 255
    va.freeformOpacity = tuple(ffo)
    SetPlotOptions(va)
    DrawPlots()
    name = SaveWindow()

sys.exit()
```

Note the really large value for samples.
This is a viz problem perfect for HPC.

Reasonable values for range command are:
range(255,5,-5) yields 51 images ~50 minutes
range(255,5,-10) yields 26 images
range(255,1,-1) yields 255 images

(13) Copy Movie_MAS_2.py and visit_python_batch_script.txt to your folder in /project/lbutler/students/your folder

VisIt batch mode



And confirm with directory listing in your terminal program.

```
[lbutler@philip1 les]$ pwd
/project/lbutler/students/les
[lbutler@philip1 les]$ ls -l
total 8
-rw-r--r-- 1 lbutler h3035 2368 Mar 28 09:56 Movie_MAS_2.py
-rwxr-xr-x 1 lbutler h3035  273 Mar 28 09:56 visit_python_batch_script.txt
```

(14a) And confirm again with file listing (more) in your terminal program.

VisIt batch mode

This should be your name

```
[lbutler@philip1 les]$ more visit_python_batch_script.txt
#!/bin/bash

#PBS -l nodes=4:ppn=8
#PBS -l walltime=00:30:00
#PBS -N visit_python
#PBS -o visit_python_output.txt
#PBS -e visit_python_error.txt
#PBS -q priority
#PBS -m e
#PBS -M lbutler@lsu.edu

cd ~
visit -cli -nowin -s /project/lbutler/students/les/Movie_MAS_2.py
```

This should be your email

This should be your name

(14b) And confirm again with file listing (more) in your terminal program.

VisIt batch mode

This should be your name

About the more command.
Press space bar to see more text.
Hit q to quit.

```
[lbutler@philip1 les]$ more Movie_MAS_2.py
import os
import sys

# Read the *.h5 data file
OpenDatabase("/project/lbutler/data_materials/MAS_rotor/MAS_rotor_cropped.h5")

# Create window attributes.
s = SaveWindowAttributes()
s.format = s.JPEG
s.outputToCurrentDirectory = 0
s.outputDirectory = "/project/lbutler/students/les"
s.fileName = "Les_volume_increase_opacity_"
s.width, s.height = 600, 400
s.screenCapture = 0
s.progressive = 1
SetSaveWindowAttributes(s)

# Create a plot
```

This should be your name

(15) Submitting the batch job.

My preference is to submit from home directory on Philip, so cd /home/lbutler

VisIt batch mode

```
[lbutler@philip1 les]$ cd /home/lbutler
[lbutler@philip1 ~]$ ls
[lbutler@philip1 ~]$ qsub /project/lbutler/students/les/visit_python_batch_script.txt
135369.philip1
[lbutler@philip1 ~]$ qstat
Job id                    Name             User            Time Use S Queue
------------------------- ---------------- --------------- -------- - -----
134321.philip1             vmd_cowX_woLigs  rcroch2                0 Q workq
134631.philip1             jobFS7.sh        michal                 0 Q workq
134784.philip1             Trib.Q10         ritt            23:16:24 R single
135174.philip1             Mnet3no          qsheng1         677:07:4 R single
135184.philip1             gb_s4_43.04      ghoshbd         00:00:00 R checkpt
135185.philip1             gb_s4_43.04      ghoshbd         00:00:00 R checkpt
135197.philip1             ...4Vx_step-2-6k sbajga2         00:00:00 R single
135220.philip1             gb_s3_29.615p    ghoshbd         00:00:00 R single
135229.philip1             STDIN            abdik           180:12:3 R workq
135231.philip1             gb_s4_25.025s7n  ghoshbd         00:00:00 R single
135232.philip1             gb_s4_43.04s0    ghoshbd         00:00:00 R single
135289.philip1             GRRMxx           wairimu         221:13:0 R workq
135297.philip1             ABC1             ritt            29:52:21 R single
135298.philip1             ABC2             ritt            29:53:10 R single
135347.philip1             Ba1.3k6step3     sbajga2                0 Q single
135352.philip1             STDIN            qsheng1         128:51:0 R single
135361.philip1             1Dnet3no         qsheng1         49:33:02 R single
135363.philip1             M1DnetDre        qsheng1                0 Q single
135369.philip1             visit_python     lbutler                0 R priority
[lbutler@philip1 ~]$
```

qsub <batch script>
showstart <job_id>
qstat
qshow <job_id>
qdelete <job_id>

(16) Checking on the batch job.

qsub <batch script>
showstart <job_id>
qstat
qshow <job_id>
qdelete <job_id>

VisIt batch mode

```
[lbutler@philip1 ~]$ qshow 135372
PBS job: 135372, nodes: 4
Hostname  Days Load CPU U# (User:Process:VirtualMemory:Memory:Hours)
philip018   77 7.93 796 17 lbutler:engine_par:267M:49M:0.0 lbutler:engine_par:1.8G:1.6G:0.0 lbutler:engine_par:267M:49M:0.0 lbutler:engine_par
:267M:49M:0.0 lbutler:engine_par:267M:49M:0.0 lbutler:engine_par:267M:49M:0.0 lbutler:engine_par:267M:49M:0.0 lbutler:engine_par:267M:49M:0.0
lbutler:pbs_demux:13M:1M lbutler:135372:63M:1M lbutler:cli:218M:12M lbutler:viewer:421M:46M lbutler:mdserver:320M:24M lbutler:mpirun:11M:1M lb
utler:hydra_pmi_proxy:11M:1M
philip019   77 0.06   0  1
philip020   77 0.00   0  1
philip021   77 0.00   0  1
```

(16) I transfered the *.jpg back to my computer

VisIt batch mode

lbutler@tezpur.hpc.lsu.edu

Local Home | History | Go To... | Reload | Info | Edit | New Folder | Delete | Disconnect | Remote Home | History

figures

Name	Size	Date
Les_volume_increase_opacity_0000.jpeg	18 KB	Mar 28 10:32
Les_volume_increase_opacity_0001.jpeg	18 KB	Mar 28 10:32
Les_volume_increase_opacity_0002.jpeg	18 KB	Mar 28 10:32
Les_volume_increase_opacity_0003.jpeg	18 KB	Mar 28 10:32
Les_volume_increase_opacity_0004.jpeg	18 KB	Mar 28 10:32
Les_volume_increase_opacity_0005.jpeg	19 KB	Mar 28 10:32
Les_volume_increase_opacity_0006.jpeg	19 KB	Mar 28 10:32
Les_volume_increase_opacity_0007.jpeg	19 KB	Mar 28 10:32
Les_volume_increase_opacity_0008.jpeg	19 KB	Mar 28 10:32
Les_volume_increase_opacity_0009.jpeg	19 KB	Mar 28 10:32
Les_volume_increase_opacity_0010.jpeg	19 KB	Mar 28 10:32
Les_volume_increase_opacity_0011.jpeg	20 KB	Mar 28 10:32
Les_volume_increase_opacity_0012.jpeg	20 KB	Mar 28 10:32
Les_volume_increase_opacity_0013.jpeg	20 KB	Mar 28 10:32
Les_volume_increase_opacity_0014.jpeg	21 KB	Mar 28 10:32
Les_volume_increase_opacity_0015.jpeg	22 KB	Mar 28 10:32
Les_volume_increase_opacity_0016.jpeg	23 KB	Mar 28 10:32
Les_volume_increase_opacity_0017.jpeg	24 KB	Mar 28 10:32
Les_volume_increase_opacity_0018.jpeg	26 KB	Mar 28 10:32
Les_volume_increase_opacity_0019.jpeg	28 KB	Mar 28 10:32
Les_volume_increase_opacity_0020.jpeg	32 KB	Mar 28 10:32

les

Name	Size	Date
Les_volume_i...ity_0023.jpeg	53 KB	Mar 28 10:23
Les_volume_i...ity_0024.jpeg	58 KB	Mar 28 10:23
Les_volume_i...ity_0025.jpeg	53 KB	Mar 28 10:23
Les_volume_i...ity_0026.jpeg	46 KB	Mar 28 10:23
Les_volume_i...ity_0027.jpeg	44 KB	Mar 28 10:24
Les_volume_i...ity_0028.jpeg	44 KB	Mar 28 10:24
Les_volume_i...ity_0029.jpeg	44 KB	Mar 28 10:24
Les_volume_i...ity_0030.jpeg	43 KB	Mar 28 10:24
Les_volume_i...ity_0031.jpeg	42 KB	Mar 28 10:25
Les_volume_i...ity_0032.jpeg	41 KB	Mar 28 10:25
Les_volume_i...ity_0033.jpeg	41 KB	Mar 28 10:26
Les_volume_i...ity_0034.jpeg	41 KB	Mar 28 10:26
Les_volume_i...ity_0035.jpeg	41 KB	Mar 28 10:27
Les_volume_i...ity_0036.jpeg	41 KB	Mar 28 10:28
Les_volume_i...ity_0037.jpeg	42 KB	Mar 28 10:28
Les_volume_i...ity_0038.jpeg	43 KB	Mar 28 10:29
Les_volume_i...ity_0039.jpeg	44 KB	Mar 28 10:29
Les_volume_i...ity_0040.jpeg	45 KB	Mar 28 10:30
Les_volume_i...ity_0041.jpeg	46 KB	Mar 28 10:30
Les_volume_i...ity_0042.jpeg	48 KB	Mar 28 10:31
Les_volume_i...ity_0043.jpeg	49 KB	Mar 28 10:32

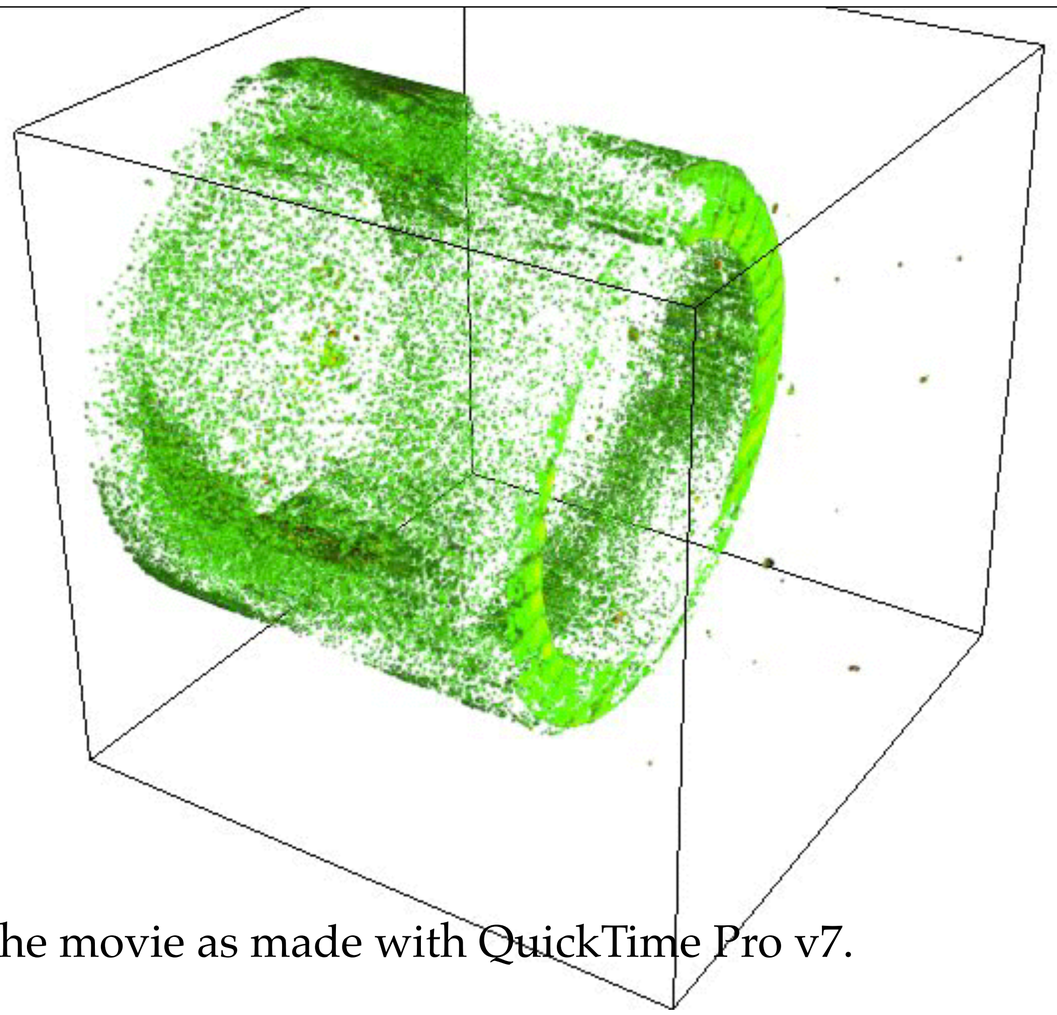
Only upto #43, and I was expecting 51. \Should have asked for more walltime. Oh well.

(17) Use any convenient program to turn *.jpg sequence into movie.

VisIt batch mode

This movie made from 44 jpg images of size 600x600.
Average file size about 40 kb. Images assembled into a movie with:

- QuickTime Pro v7
- GraphicConverter v6.6, and
- iMovie '08



The movie as made with QuickTime Pro v7.

```
resampleTarget = 50000000
opacityMode = va.FreeformMode
PlotOptions(va)

raw the Plot
wPlots()

# Set the plot orientation
v0 = GetView3D()
v0.viewNormal = (0.80, 0.5, -0.50)
SetView3D(v0)
# print v0
```

Recall this comment about the loop parameters:
range(255,5,-5) yields 51 images ~15 minutes
range(255,5,-10) yields 26 images
range(255,1,-1) yields 255 images

```
# Loop over a range of opacity values and save the plots
for j in range(255,5,-5):
    ffo = range(0,256)
    for i in ffo:
        if i <= j:
            ffo[i] = 0
        else:
            ffo[i] = 255
    va.freeformOpacity = tuple(ffo)
    SetPlotOptions(va)
    DrawPlots()
    name = SaveWindow()
```