Workshop: High-performance computing for economists

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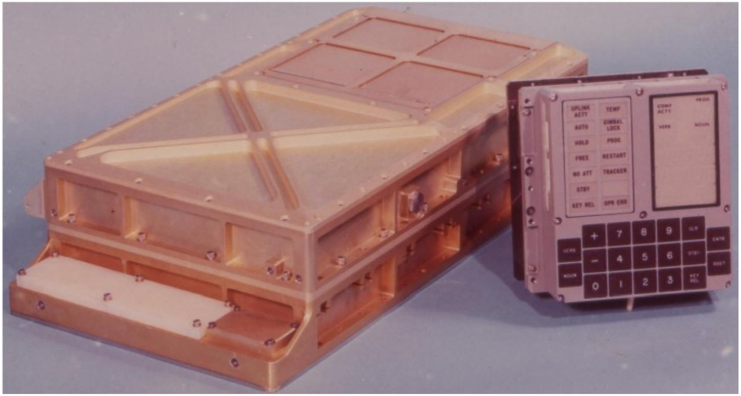
August 18-21, 2014: Day 1

Workshop: High-performance computing for economists

HPC

Back in the days...



HPC

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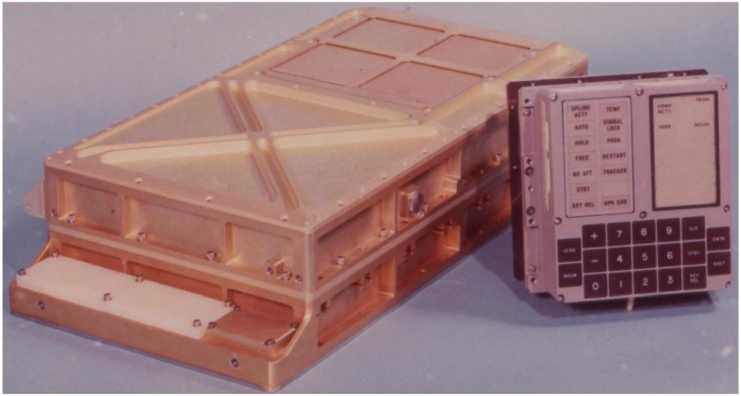
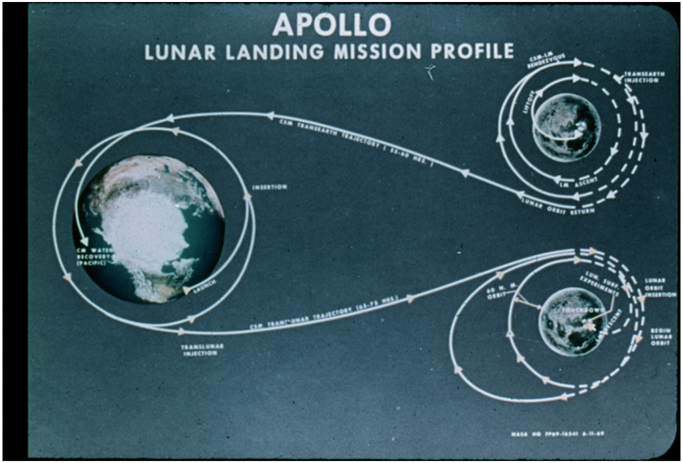


RAM: 2,000 words (2kB); Speed: 2 MHz
Source: Wikipedia

They went to the moon



Source: Flickr

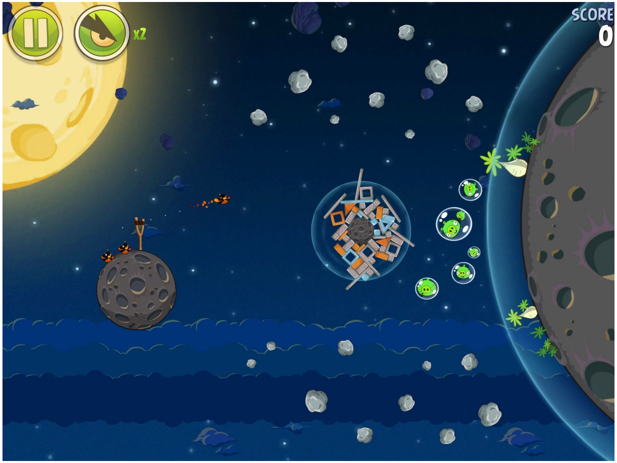
Big progress

RAM: 2 $\times$32 kB; Speed: 1 MHz, $1,500 (today's USD)
Wikipedia

Today

RAM: 2 $\times 1024^2$ kB; Speed: 1.700 MHz $\times$ 4
$700 (today's USD) Source: Wikipedia

We still fly to the moon



Source CNET

This is where you can go

Stampede (no. 6 on Top500 as of June 2013)

This is where you can go

Stampede (no. 6 on Top500 as of June 2013)

RAM: 192 $\times 1024^3$ kB, Speed: 2,700 Mhz $\times$ 462,462

Source: TACC

But first...

But first...

http://viewfromwitsend.wordpress.com/

What do you learn in a Ph.D. program?

What do you learn in a Ph.D. program?

How to learn...

Goal of this class

Goal of this class

To open new doors, to be able to conceive of problems that you didn't think had a feasible solution.

Goal of this class

To open new doors, to be able to conceive of problems that you didn't think had a feasible solution.
To broaden your knowledge about what you do NOT know

Overview

Day 1

- Programming basics (Lars)

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- Programming basics (Lars)
    - Choosing an editor

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  - How to structure programs, texts, etc.

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  - NX, SSH, Linux, request an account on cluster

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- Subroutines: the example of function programming in R (Lars)

Overview

Day 2

Overview

Day 3

Structure of the class

Teaching...

We'll take you on a 4,000 m flight through topics...

Structure of the class

Teaching...

We'll take you on a 4,000 m flight through topics...

... and practice

... and then swoop in on some examples, leaving ample time to practice it.

Choosing editors

Why does choosing editors matter?

The (applied) research process iterates through writing papers and doing estimation. You want to use the appropriate tools for each task.

Integrated or separate

- You can use native tools that come with each word processing facility/programming language/etc.
- Not all of them will have one.
- Not all of them will work on all platforms.
- You will likely use multiple tools

Choosing an editor

... or system

Separate editors and systems

- MS Word and math editor (Windows/OSX but compatibility issues)
- LibreOffice (Windows/OSX/Linux but not as good)
- NotePad++ (Windows)
- Gedit, (X)Emacs, Kate (Linux)
- ?? (OSX)

LaTeX: all platforms, but some GUIs are not cross-platform, ease of use varies:

- TeXstudio (all platforms)
- TeXMaker (all platforms)
- Scientific Workplace (Windows, mythical Linux)
- TeXWorks+Miktex
- TEXnicCenter
- and (many more)

Choosing an editor

... or system

Integrating programming and running

- IDE (Eclipse, ActiveState Komodo, etc.)
- Native programming GUIs (SAS, Matlab, Stata)
- Gedit, (X)Emacs (with add-on functionality)

Integrating programs and text/results

- SWeave (integrates LaTeX and R)
- RStudio (GUI to R and SWeave)
- StatRep (Integrated SAS and LaTeX, Source 1, Source 2)

Structuring programs

Easy...

Listing 1: mystuff.sas

```
data "C:\Users\Me\CensusChina.sas7bdat";
      set "C:\Users\Me\CensusChina.sas7bdat";
      earn=log(earn);
run;
proc reg data="C:\Users\Me\CensusChina.sas7bdat";
model earn = sex education experience;
run;
```

What can possibly be wrong about that?

Structuring programs 2

Easier...

Listing 2: mystuff.do

```
use "C:\Users\Me\CensusChina.dta"
replace earn=log(earn)
regress earn sex education experience
save, replace
```

What can possibly be wrong about that?

Structuring programs 3

Actually...

Everything!

- Name of program: uninformative
- Destruction of original data: program cannot be re-run for same results
- No portability: cannot be run anywhere else
- No explanation: why are we doing this?

But of course, nobody does that, right?

Structuring programs 4

Better...?

Listing 3: china-regression.sas

```
data logCensusChina;
    set "C:\Users\Me\CensusChina.sas7bdat";
    earn=log(earn);
run;
proc reg data=logCensusChina;
model earn = sex education experience;
run;
```

Structuring programs 4

Better...?

Listing 4: china-regression.sas

```
data logCensusChina;
    set "C:\Users\Me\CensusChina.sas7bdat";
    earn=log(earn);
run;
proc reg data=logCensusChina;
model earn = sex education experience;
run;
```

Somewhat...

Structuring programs 5

Addressing these issues

- Naming of programs: here
- Commenting: here
- Versioning: up next
- Portability and Data management: tomorrow

Key notions about naming

Think of yourself as highly amnesiac...

- The research paper you are writing now will be submitted, rejected, worked on, questioned...

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Key notions about naming

Think of yourself as highly amnesiac...

- The research paper you are writing now will be submitted, rejected, worked on, questioned...
- ... by others and yourself
- ... in intervals of weeks, months, years...
- Your future research assistant and the future YOU will need to understand how to go through it.

Naming

The really bad

```
mystuff.R
read.R
version2.R
ols.sas
```

Naming

The really bad

```
mystuff.R
read.R
version2.R
ols.sas
```

The bad

```
readCensus.R
readBLS.R
prepareCensus.R
runOLS.sas
```

Naming

Better

```
01_readBLS.R
02_readCensus.R
03_prepareCensus.R
04_create_analysis_data.R
05_runOLS.sas
```

Naming

Better

```
01_readBLS.R
02_readCensus.R
03_prepareCensus.R
04_create_analysis_data.R
05_runOLS.sas
```

Even better

```
01_01_readBLS.R
02_01_readCensus.R
02_02_prepareCensus.R
03_01_create_analysis_data.R
04_01_runOLS.sas
README.txt
```

Naming

Going overboard?

```
icf/ctrlprogs/control_icf.sas
icf/ctrlprogs/parameters_icf.sas
icf/library/macros/icf_cleanup.sas
icf/library/macros/icf_impute_county_res.sas
icf/library/macros/licf_findnum.sas
icf/library/macros/licf_proxy.sas
icf/library/macros/licf_stars1.sas
icf/library/macros/licf_tgrlatlongs.sas
icf/library/sasprogs/01_icfqa.sas
icf/library/sasprogs/01_icf.sas
icf/library/sasprogs/02_icfqa.sas
icf/library/sasprogs/02_icf.sas
icf/library/sasprogs/03_icfqa.sas
icf/library/sasprogs/03_icf.sas
[snip]
icf/library/sasprogs/19_icf.sas
```

Naming

Going overboard?

```
icf/ctrlprogs/control_icf.sas
icf/ctrlprogs/parameters_icf.sas
icf/library/macros/icf_cleanup.sas
icf/library/macros/icf_impute_county_res.sas
icf/library/macros/licf_findnum.sas
icf/library/macros/licf_proxy.sas
icf/library/macros/licf_stars1.sas
icf/library/macros/licf_tgrlatlongs.sas
icf/library/sasprogs/01_icfqa.sas
icf/library/sasprogs/01_icf.sas
icf/library/sasprogs/02_icfqa.sas
icf/library/sasprogs/02_icf.sas
icf/library/sasprogs/03_icfqa.sas
icf/library/sasprogs/03_icf.sas
[snip]
icf/library/sasprogs/19_icf.sas


ehf/ctrlprogs/control_ehf.sas
ehf/library/macros/read_bls.sas
ehf/library/sasprogs/01_ehf.sas
[snip]
```

Naming

With minor modification

```
icf/ctrlprogs/control_icf.sas
icf/ctrlprogs/parameters_icf.sas
icf/library/macros/icf_cleanup.sas
icf/library/macros/icf_impute_county_res.sas
icf/library/macros/licf_findnum.sas
icf/library/macros/licf_proxy.sas
icf/library/macros/licf_stars1.sas
icf/library/macros/licf_tgrlatlongs.sas
icf/library/sasprogs/01_icf.sas
icf/library/sasprogs/02_icf.sas
icf/library/sasprogs/03_icf.sas
[snip]
icf/library/sasprogs/19_icf.sas
icf/library/sasprogs/01_icfqa.sas
icf/library/sasprogs/02_icfqa.sas
icf/library/sasprogs/03_icfqa.sas
```

Can you figure out in what sequence to run them?

Linux

- used on most compute clusters
- used on very few desktop computers
- but...

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Bash

- bash is a “shell” - a text interface command interpreter
- bash or ksh (Korn shell) or csh (C-shell) are the most common
- bash is available on Linux and

Linux

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Bash

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- bash or ksh (Korn shell) or csh (C-shell) are the most common
- bash is available on Linux and OSX
- you can also download Cygwin, getting bash for Windows

Access to your local compute cluster

Several on-campus compute resources

- Cornell Center for Advanced Computing (CAC)

Access to your local compute cluster

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- Cornell Center for Advanced Computing (CAC)
- Cornell Institute for Social and Economic Research (CISER)

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- Cornell Center for Advanced Computing (CAC) $\rightarrow$ Thursday
- Cornell Institute for Social and Economic Research (CISER)$\rightarrow$ Thursday

Access to your local compute cluster

Several on-campus compute resources

- Cornell Center for Advanced Computing (CAC) $\rightarrow$ Thursday
- Cornell Institute for Social and Economic Research (CISER)$\rightarrow$ Thursday
- Economics Compute Cluster Organization (ECCO), aka Social Science Gateway (SSG)

Getting access to ECCO

You already have...

- You have an account by virtue of participating in this class
- Moving forward, you will be eligible to faculty-sponsored accounts
- Currently soft-monitoring of resource usage

Getting access to ECCO

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Have you logged in via SSH to reset your password?

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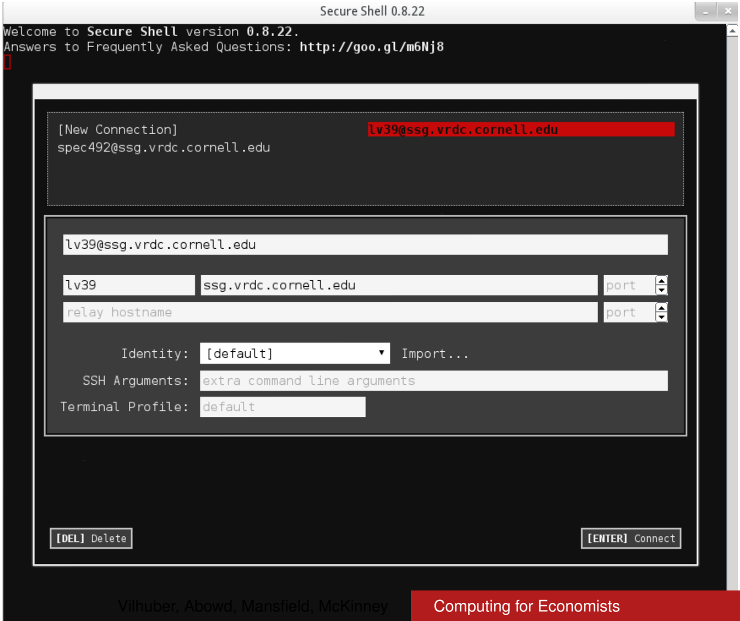
... but do you have **access**?

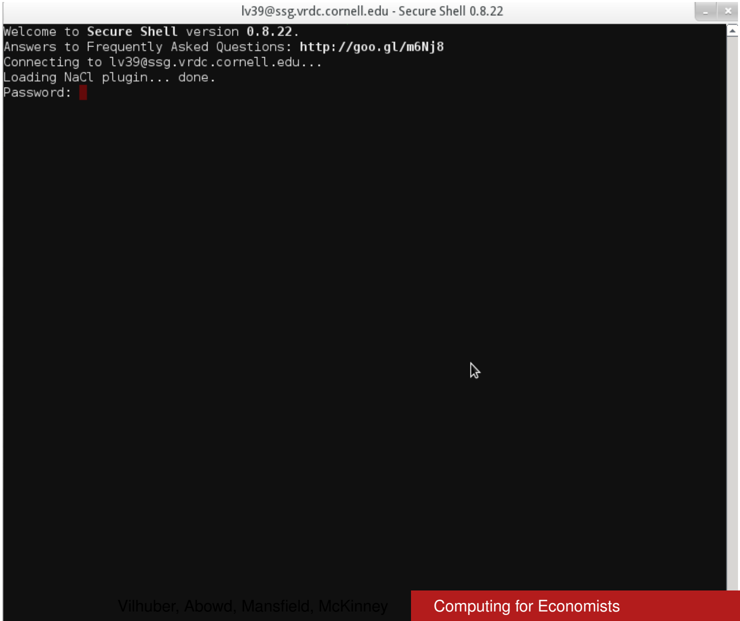
Have you logged in via SSH to reset your password?
$\rightarrow$ Instructions

Quick walkthrough, using Chrome SSH



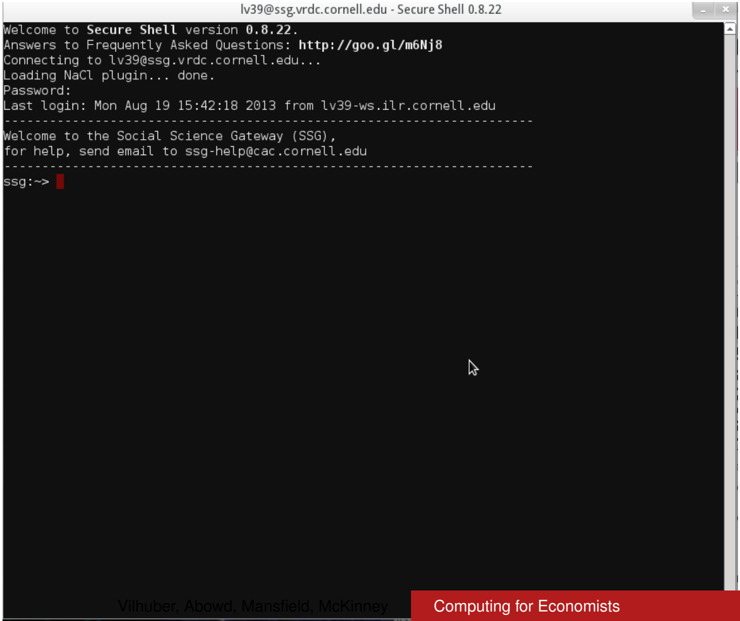
```
Secure Shell 0.8.22
Welcome to Secure Shell version 0.8.22.
Answers to Frequently Asked Questions: http://goo.gl/m6Nj8

[New Connection]                    lv39@ssg.vrdc.cornell.edu
spec492@ssg.vrdc.cornell.edu

lv39@ssg.vrdc.cornell.edu

lv39        ssg.vrdc.cornell.edu        port
relay hostname                          port

        Identity: [default]     Import...
   SSH Arguments: extra command line arguments
Terminal Profile: default

[DEL] Delete                            [ENTER] Connect
```

Quick walkthrough, using Chrome SSH



```
Welcome to Secure Shell version 0.8.22.
Answers to Frequently Asked Questions: http://goo.gl/m6Nj8
Connecting to lv39@ssg.vrdc.cornell.edu...
Loading NaCl plugin... done.
Password:
```

Quick walkthrough, using Chrome SSH


lv39@ssg.vrdc.cornell.edu - Secure Shell 0.8.22

```
Welcome to Secure Shell version 0.8.22.
Answers to Frequently Asked Questions: http://goo.gl/m6Nj8
Connecting to lv39@ssg.vrdc.cornell.edu...
Loading NaCl plugin... done.
Password:
Last login: Mon Aug 19 15:42:18 2013 from lv39-ws.ilr.cornell.edu
----------------------------------------------------------------------
Welcome to the Social Science Gateway (SSG),
for help, send email to ssg-help@cac.cornell.edu
----------------------------------------------------------------------
ssg:~>
```

Why SSH?

Most compute clusters have ONLY SSH access

It is thus worthwhile to learn enough about it here, in order to be functional there: CAC “Red Cloud”, Amazon Cloud, XSEDE.

Linux rules... the HPC world

All 10 of the top 10 TOP500 computers run Linux (as the compiler front-end, if not compute OS)

Graphical access

Two types of graphical access

- with an “X server” (native in Linux, optional in Windows and OSX)

Graphical access

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Graphical access

Two types of graphical access

- with an “X server” (native in Linux, optional in Windows and OSX) $\rightarrow$ standard way on most clusters
- using NX client software for improved experience

Access via NX

What is NX?

NX is software similar to Windows Remote Desktop, allowing for a graphical interface to be made available remotely.

- Client is free (provided by Nomachine)
- We use a free server (not provided by Nomachine, but fully functional)
- Clients can be launched by installing dedicated client (all OS) or by launching the webclient (currently not working for some Linux)

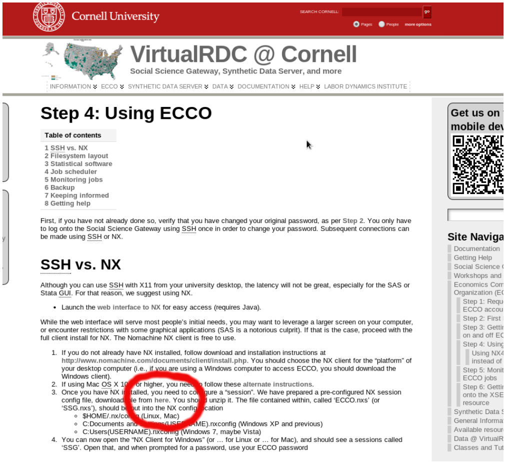
Important note

NX on ECCO security

You MUST download the custom-configured session from the VRDC website; the default session configuration from the NX client install will not work.

Details: we use a custom SSH key for the NX client, for some minimal additional security.

Important note



Step 4: Using ECCO

Table of contents

First, if you have not already done so, verify that you have changed your original password, as per Step 2. You only have to log onto the Social Science Gateway using SSH once in order to change your password. Subsequent connections can be made using SSH or NX.

SSH vs. NX

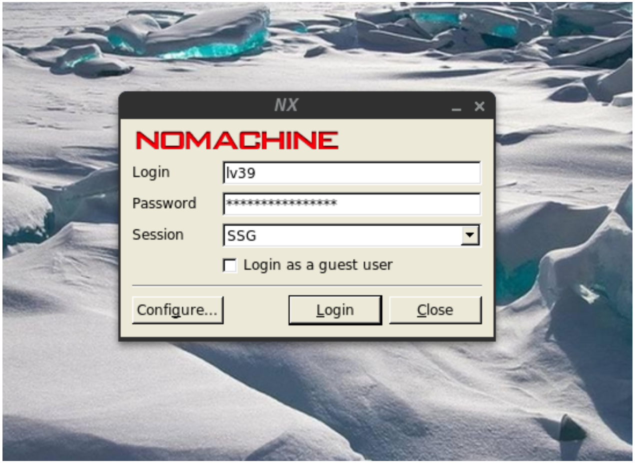
Although you can use SSH with X11 from your university desktop, the latency will not be great, especially for the SAS or Stata GUI. For that reason, we suggest using NX.

- Launch the web interface to NX for easy access (requires Java).

While the web interface will serve most people's initial needs, you may want to leverage a larger screen on your computer, or encounter restrictions with some graphical applications (SAS is a notorious culprit). If that is the case, proceed with the full client install for NX. The Nomachine NX client is free to use.

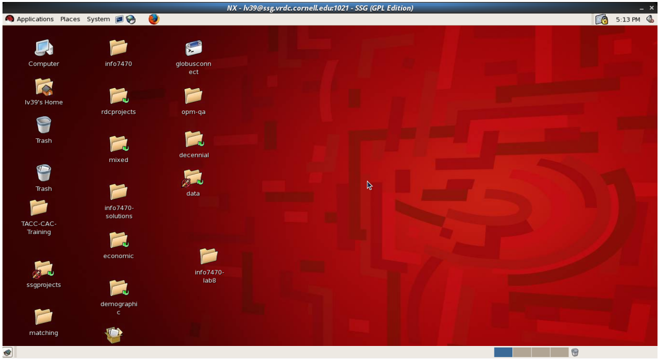
1. If you do not already have NX installed, follow download and installation instructions at http://www.nomachine.com/documents/client/install.php. You should choose the NX client for the "platform" of your desktop computer (i.e., if you are using a Windows computer to access ECCO, you should download the Windows client).
2. If using Mac OS X 10[illegible] or higher, you need to follow these alternate instructions.
3. Once you have NX installed, you need to configure a "session". We have prepared a pre-configured NX session config file, downloadable from here. You should unzip it. The file contained within, called 'ECCO.nxs' (or 'SSG.nxs'), should be put into the NX config location
   - $HOME/.nx/config (Linux, Mac)
   - C:Documents and Settings(USERNAME).nxconfig (Windows XP and previous)
   - C:Users(USERNAME).nxconfig (Windows 7, maybe Vista)
4. You can now open the "NX Client for Windows" (or … for Linux or … for Mac), and should see a sessions called 'SSG'. Open that, and when prompted for a password, use your ECCO password

Logging on



Login lv39
Password ******************
Session SSG
☐ Login as a guest user

Successful connection



Basic Linux, basic scripting

Why worry?

You will end up doing something on the command line

- Launch a program from a compute-cluster job

Why worry?

You will end up doing something on the command line

- Launch a program from a compute-cluster job
- Launch a job submission

Why worry?

You will end up doing something on the command line

- Launch a program from a compute-cluster job
- Launch a job submission
- Basic scripting

Linux in 2 minutes

- ls - will list the contents of a directory
- cd - will “change directory”
- cd .. (note the spaces) will go up a directory
- cd (name) will go into the directory (name)
- rm (name) will delete
- mkdir (name) will create a directory called (name)
- vi (name) will open a venerable command line editor for file (name)

Linux in 2 minutes

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- vi (name) will open a venerable command line editor for file (name) (CAUTION: to exit, hit ESC, then :q!)

Basic scripting in Linux

A basic loop on the command line

```
for (( i; i<10; i++ ))
do
  echo $i
done
for i in 1 3 7 99
do
  echo $i
done
```

Source: [1]

Capturing output

You can capture the output from a command

```
> seq 1 3
1
2
3
```

Now let's use that:

```
for i in $(seq 1 3)
do
  echo $i
done
```

Basic scripting in Linux

Use for practical things

Remember that ICF program sequence? How would we go about starting 19 programs in sequence?

```
for program in $(ls *_icf.sas)
do
  sas $program
done
```

Advanced linux in 2 minutes

The gateway to everything

man

or try http://www.linuxmanpages.com or http://linux.die.net/man/

The toolkit

- sed
- grep
- awk
- regex (regular expressions)

Advanced scripting in Linux

Use for practical things

What if I'm running 100s of programs, and trying to figure out if any of them have errors?

```
for logfiles in $(ls *_icf.log)
do
  grep ERROR $logfiles
done
```

Now let's try it out

Next section

Next section