Workshop: High-performance computing for economists

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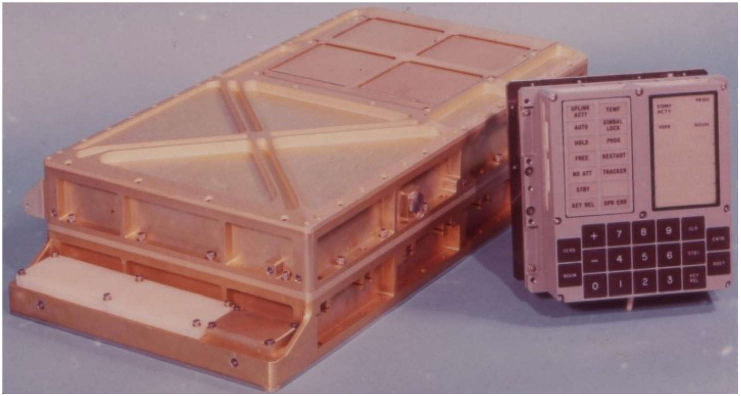
Workshop: High-performance computing for economists

HPC

Back in the days...



HPC

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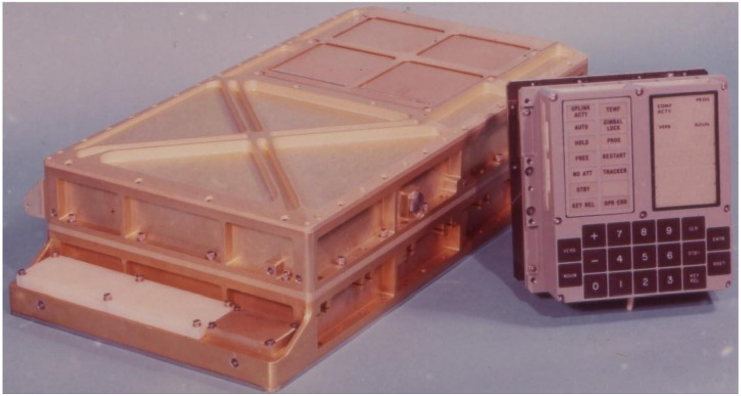
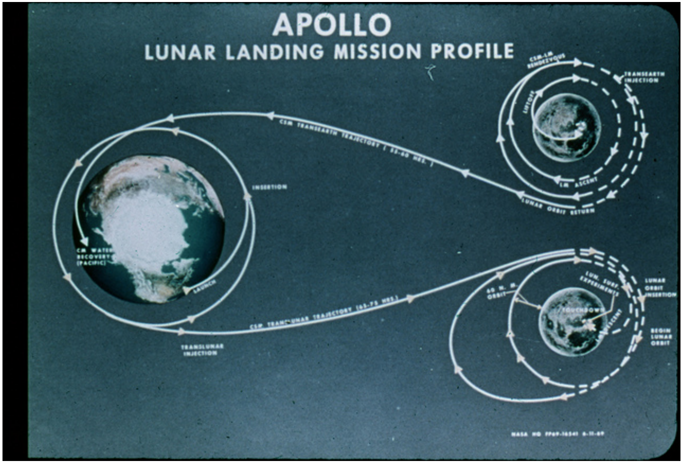


RAM: 2,000 words (2kB); Speed: 2 MHz
Source: Wikipedia

They went to the moon



Source: Flickr

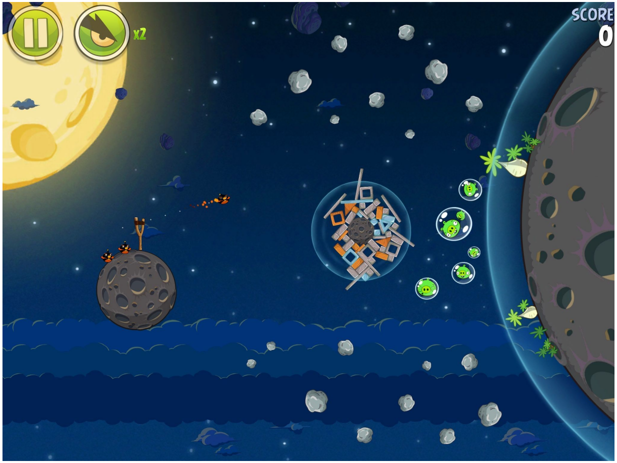
Big progress

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...

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http://viewfromwitsend.wordpress.com/

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

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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

So in order to do that...

So in order to do that...

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Overview

Day 1

- Programming basics (Lars)

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  - Choosing an editor

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- HP resources at Cornell, elsewhere

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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)
- Sublime Text (OSX)
- Atom (all, see also MS Visual Studio Code)

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/knitr (integrates LaTeX and R)
- RStudio (GUI to R and SWeave/knitr)
- Shiny (web interface to R with dynamic results)
- StatRep (Integrated SAS and LaTeX, Source 1, Source 2)

Structuring programs

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?

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)

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- 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

Basic Linux, basic scripting

Why worry?

You will end up doing something on the command line

- Launch a program from a compute-cluster job

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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)

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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