

# Running Applications on the Hoffman2 Cluster: An Introduction

Doing research on the Hoffman2 cluster

Raffaella D'Auria, PhD

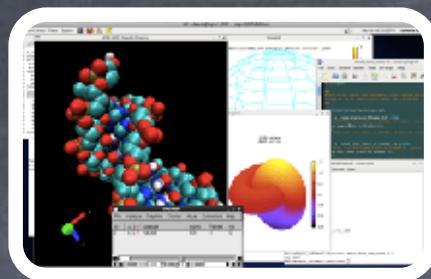
## Learning outcomes:

- what is the Hoffman2 cluster
- getting an account on Hoffman2
- connecting to the Hoffman2 cluster w/ X11-forwarding enabled (from different OSs)
- copying your data to and from Hoffman2
- unix command line survival quick & dirty guide
- getting an interactive session
- how to find out what applications are on Hoffman2?
- loading/unloading applications in your environment
- install/compile your application
- run a batch job

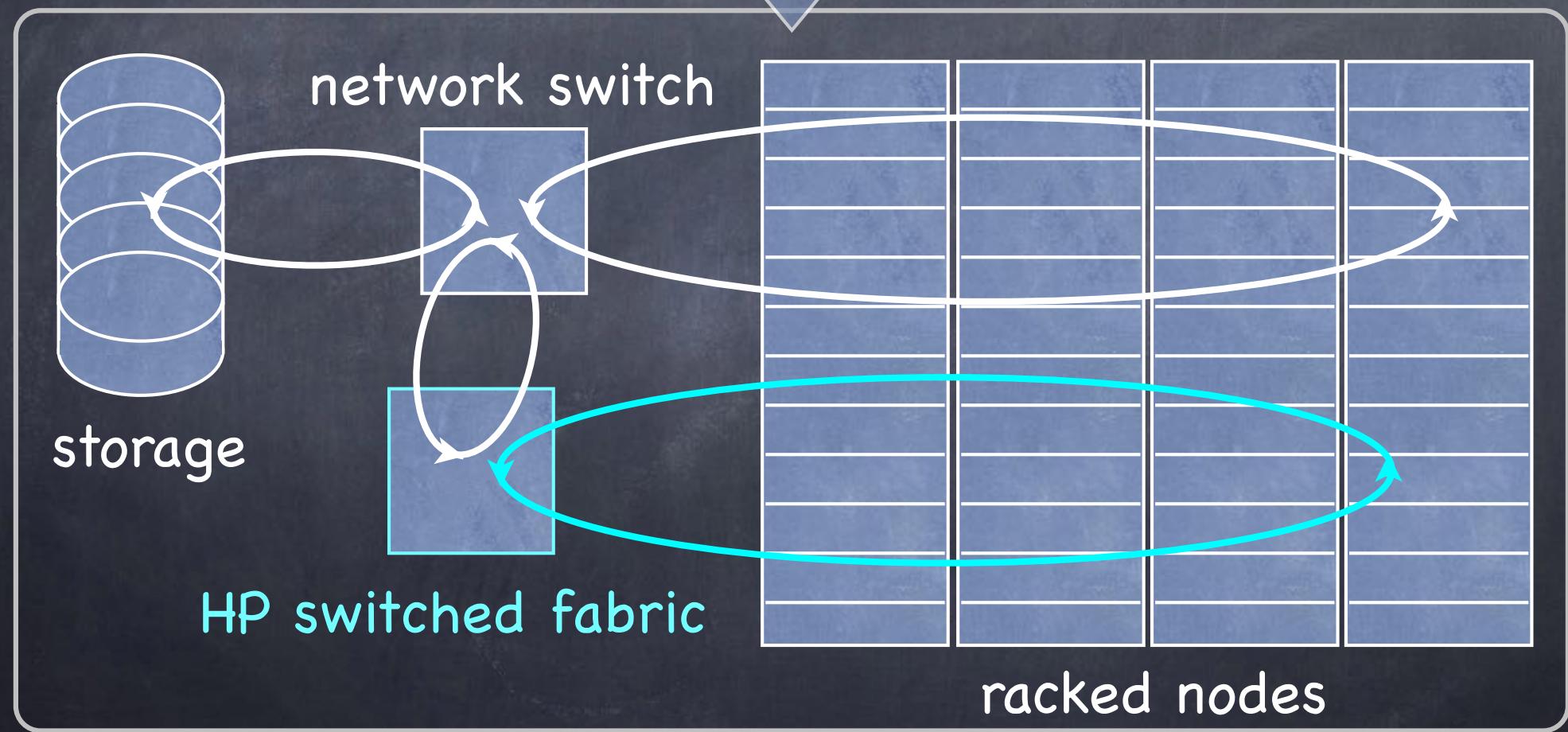


# The Hoffman2 cluster

User running  
applications



Hoffman2 cluster



https://www.hoffman2.idre.ucla.edu

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UCLA Hoffman2 Cluster User Guide

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## Getting Started

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[New User Registration](#) <- Click here to apply for an account on a cluster hosted by IDRE.

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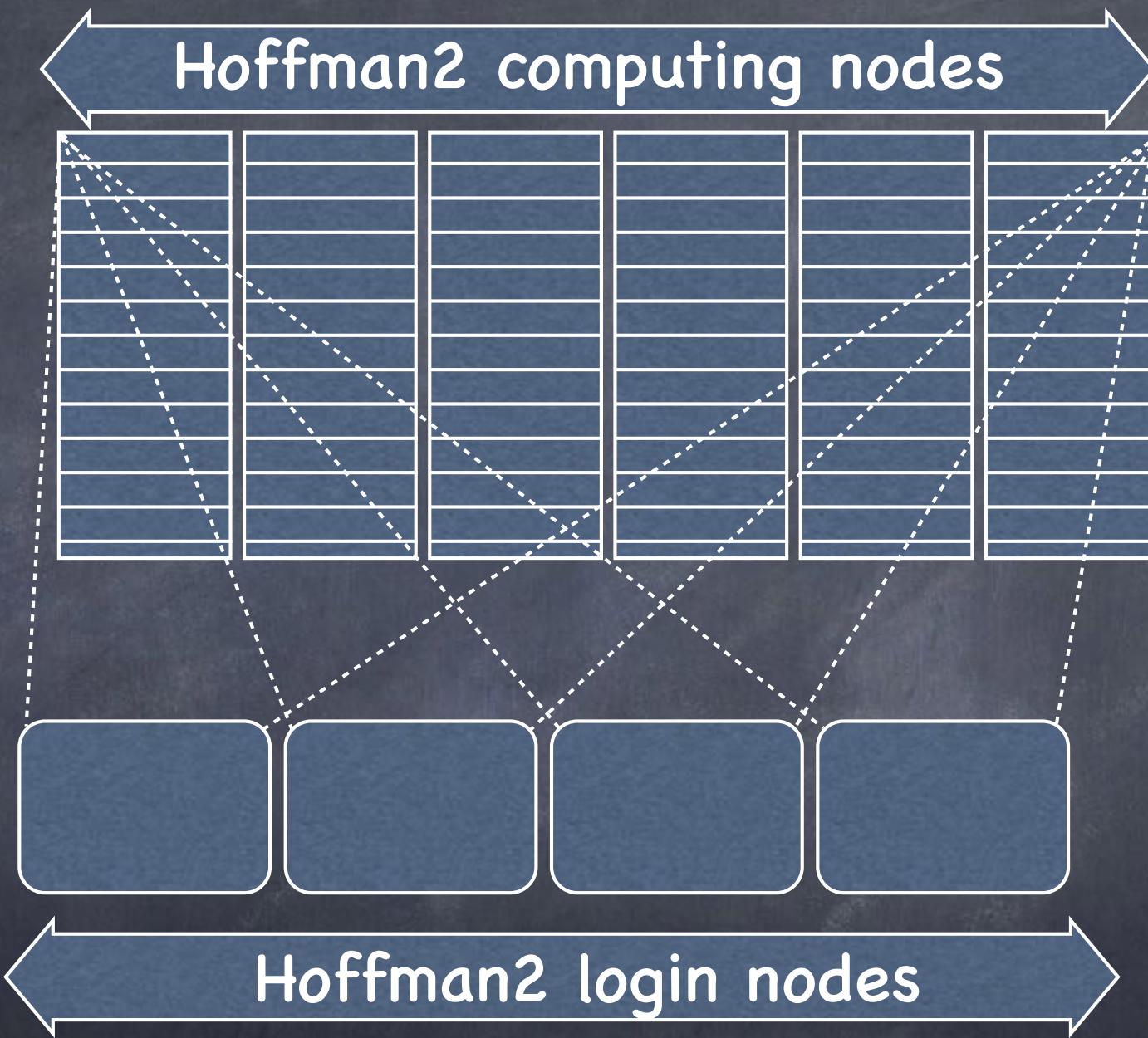
[Your Grid account](#)

[Faculty Sponsor information](#)

Who is eligible for an account on a cluster hosted by IDRE? Find out on the [Security Policy](#) page. All accounts on any cluster hosted by IDRE are governed by the Security Policy. Read it.

- [New User Registration](#)
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- [Your Grid account](#)
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## Accessing the Hoffman2 Cluster

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You can connect to the Hoffman2 cluster using the SSH protocol. For command line-type operations, that do not require opening of graphical interfaces, using SSH will suffice. To allow on your local computer opening of graphical interfaces (GUI applications) running on the cluster you will need to allow forwarding of the X Window System over SSH. NX is an alternative way to connect to the cluster that allows opening of a remote desktop on the cluster (with access to graphical interfaces). You can also connect to the Hoffman2 cluster via ipython notebooks.



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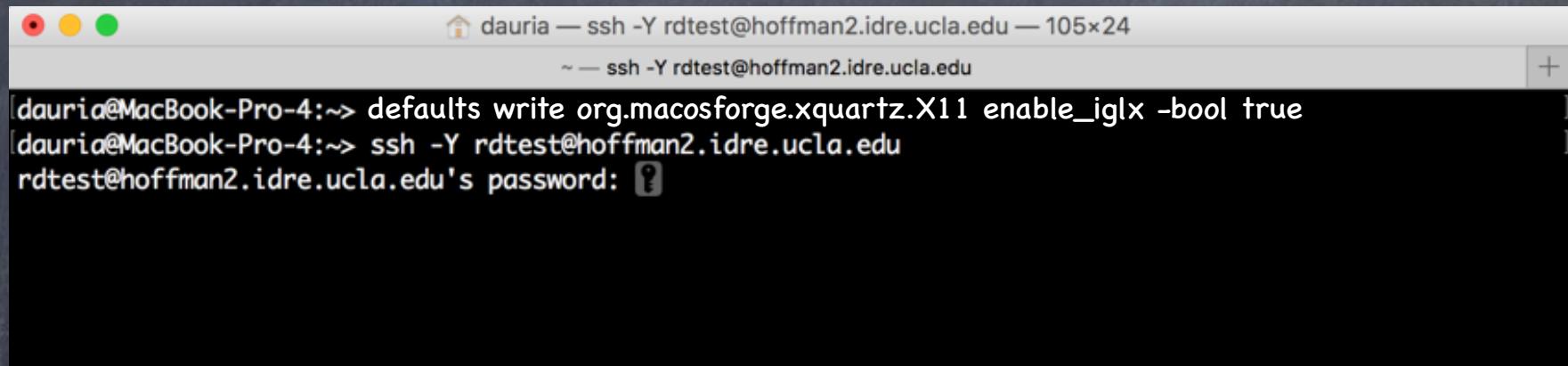
[Notes for Xming users](#)

[Notes for Cygwin users](#)

[Use NX as an alternative on a slow network](#)

You can run interactive applications that have Graphical User interfaces (GUI) by connecting to the cluster login node using ssh with X11 Forwarding enabled. Your local machine must be running an X server and enable X11 forwarding in order to display graphical output.

# Connecting to the Hoffman2 Cluster from a Unix-like environment (Linux, OSX, MacOS, etc.)



```
dauria — ssh -Y rdtest@hoffman2.idre.ucla.edu — 105x24
~ — ssh -Y rdtest@hoffman2.idre.ucla.edu
[dauria@MacBook-Pro-4:~] defaults write org.macosforge.xquartz.X11 enable_iglx -bool true
[dauria@MacBook-Pro-4:~] ssh -Y rdtest@hoffman2.idre.ucla.edu
rdtest@hoffman2.idre.ucla.edu's password:
```

## Notes for XQuartz users

Indirect GLX was disabled by default in Xorg 1.17, starting from XQuartz version 2.7.9, to enable Indirect GLX and to allow remote visualization on the cluster you will have to issue at the terminal command prompt of your mac:

`defaults write org.macosforge.xquartz.X11 enable_iglx -bool true`

See [About X11 and OS X Mountain Lion](#) from <http://support.apple.com/kb/HT5293>. For Mac OS X 10.4 (Tiger): X11 should be installed from the OS media and manually started.



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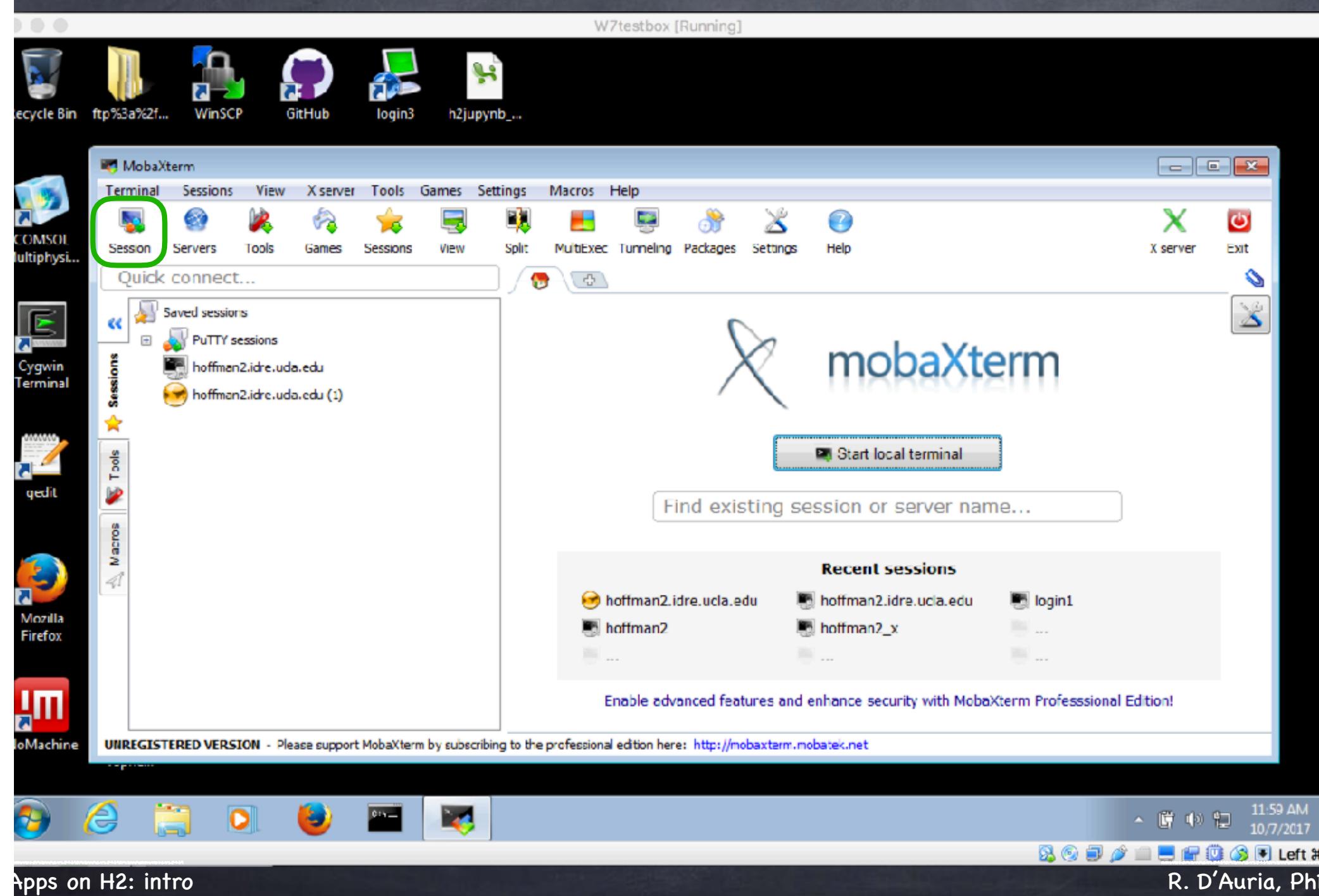
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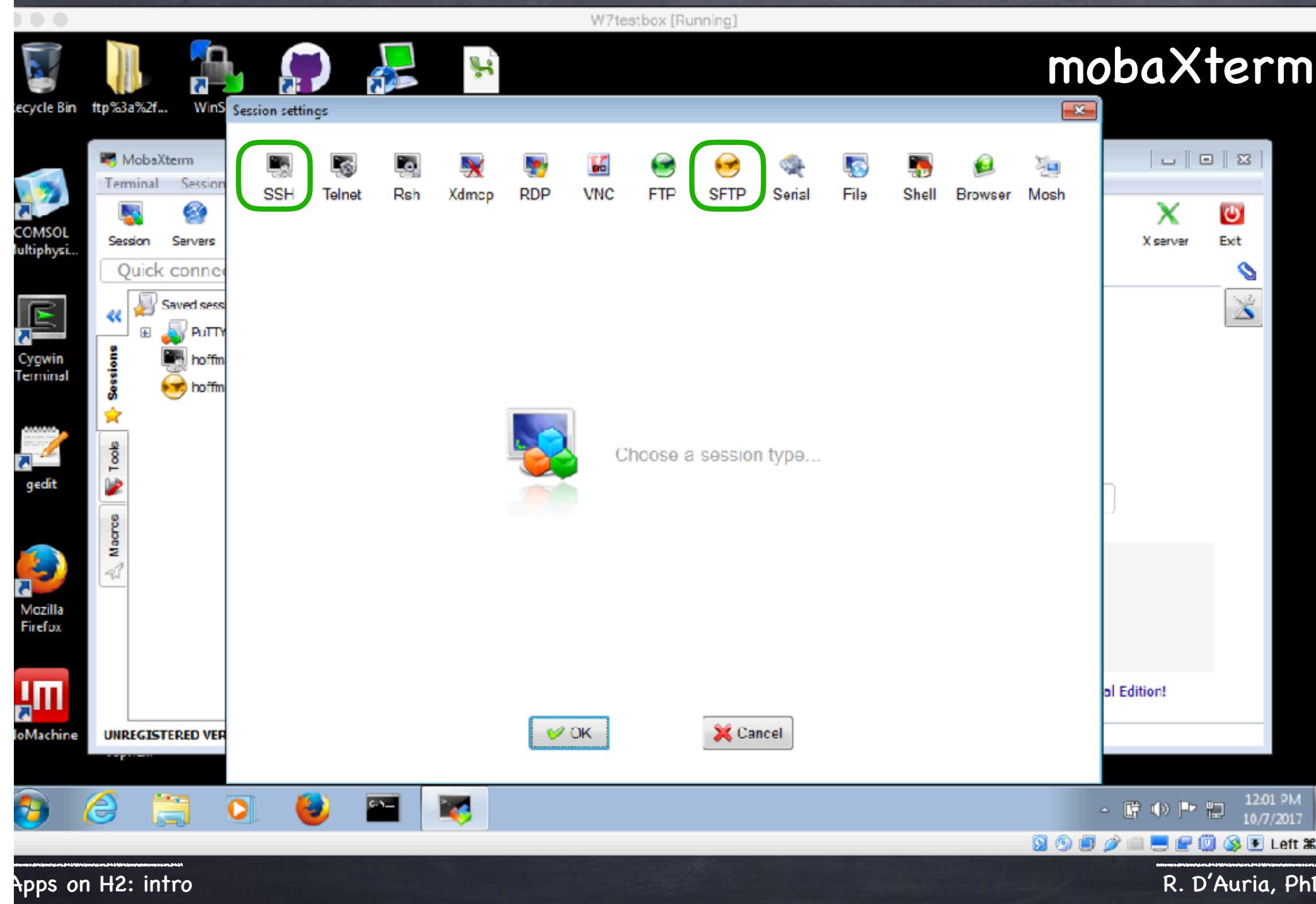
[Use NX as an alternative on a slow network](#)

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# Connecting to the Hoffman2 Cluster from Windows box

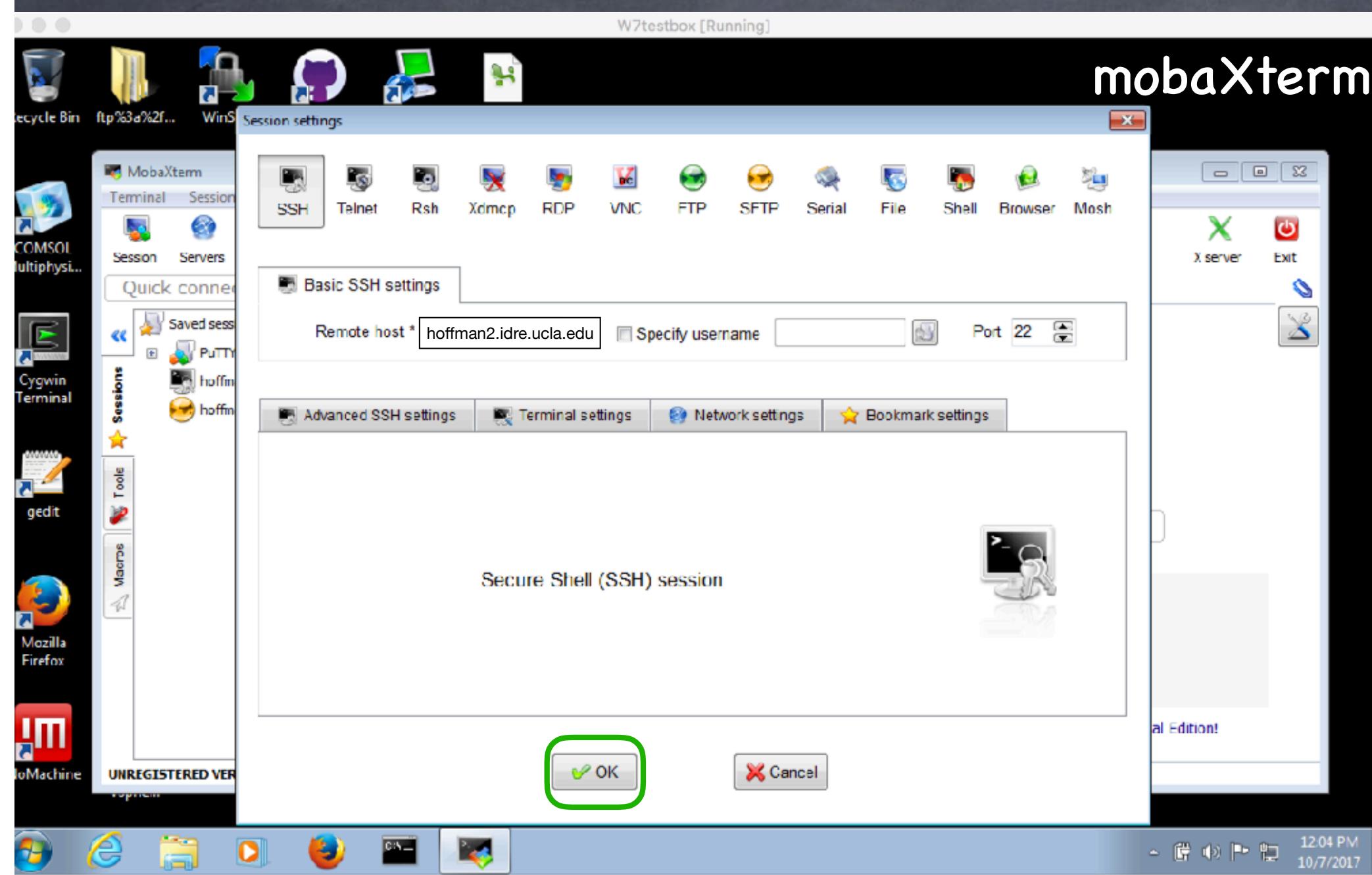


# Connecting to the Hoffman2 Cluster from Windows box



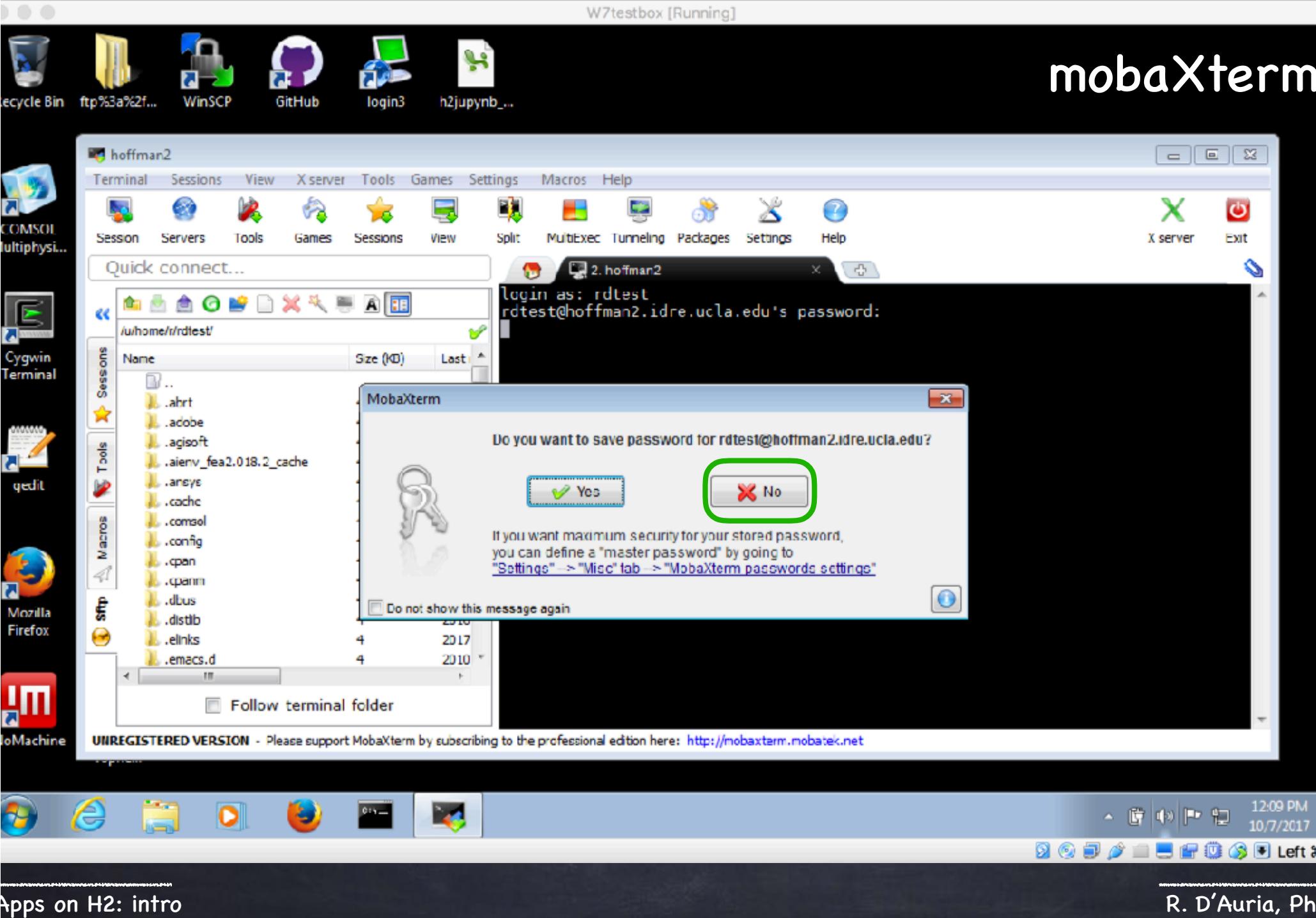
# Connecting to the Hoffman2 Cluster from Windows box

mobaXterm

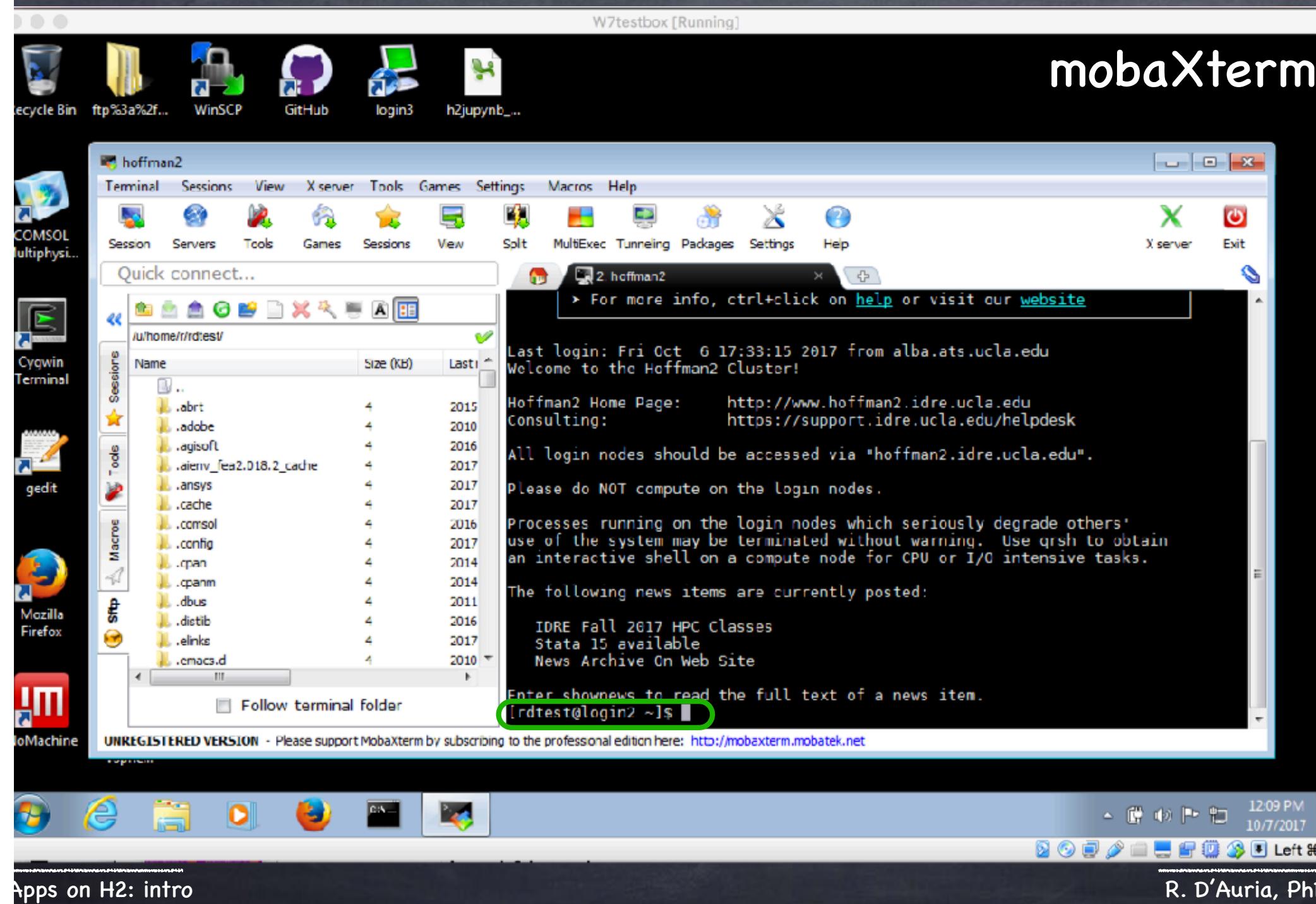


# Connecting to the Hoffman2 Cluster from Windows box

mobaXterm



# Connecting to the Hoffman2 Cluster from Windows box





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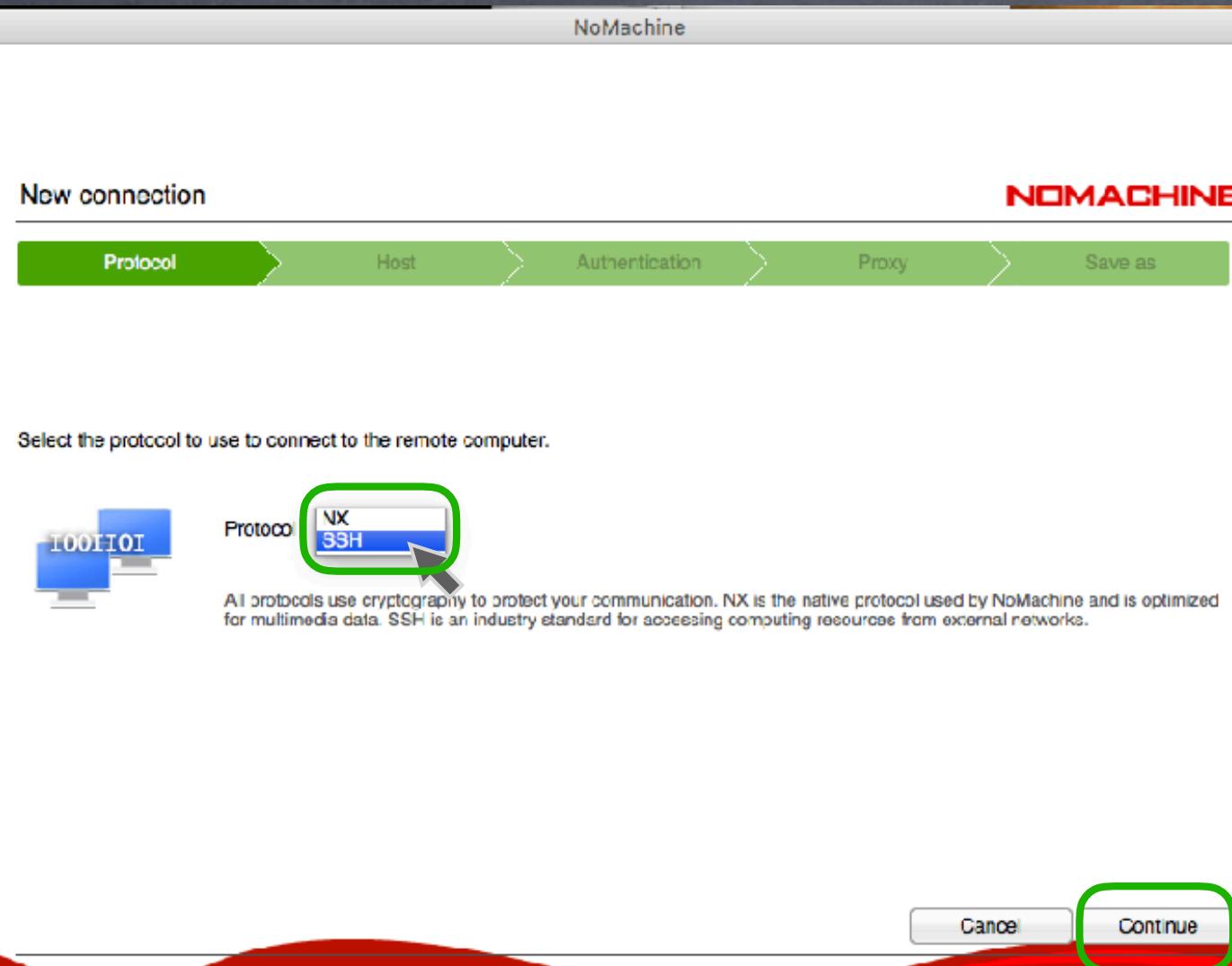
[Notes for Xming users](#)

[Notes for Cygwin users](#)

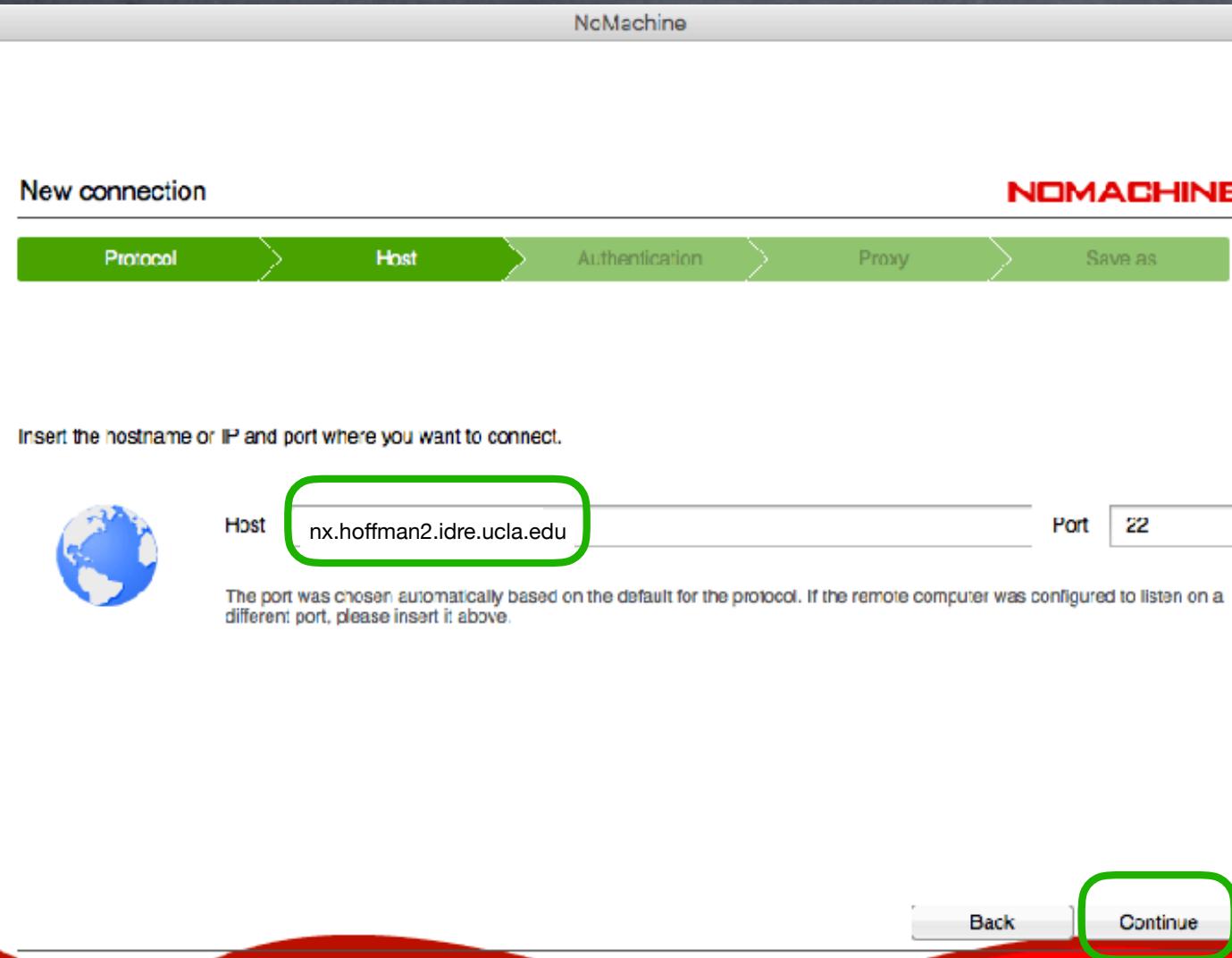
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# Connecting to the Hoffman2 Cluster via NX



# Connecting to the Hoffman2 Cluster via NX



# Connecting to the Hoffman2 Cluster via NX

The screenshot shows the 'New connection' wizard interface for NoMachine. The title bar says 'NcMachine'. The top navigation bar has tabs: Protocol, Host, Authentication (which is highlighted in green), Proxy, and Save as. The main content area asks 'How do you want to authenticate on the host?'. It shows two options: 'Use the system login' (selected, indicated by a blue radio button) and 'Use the NoMachine login' (indicated by a grey radio button). A green rounded rectangle highlights the 'Use the system login' section. At the bottom right, there are 'Back' and 'Continue' buttons, with 'Continue' being highlighted by a green rectangle.

New connection

NOMACHINE

Protocol > Host > **Authentication** > Proxy > Save as

How do you want to authenticate on the host?

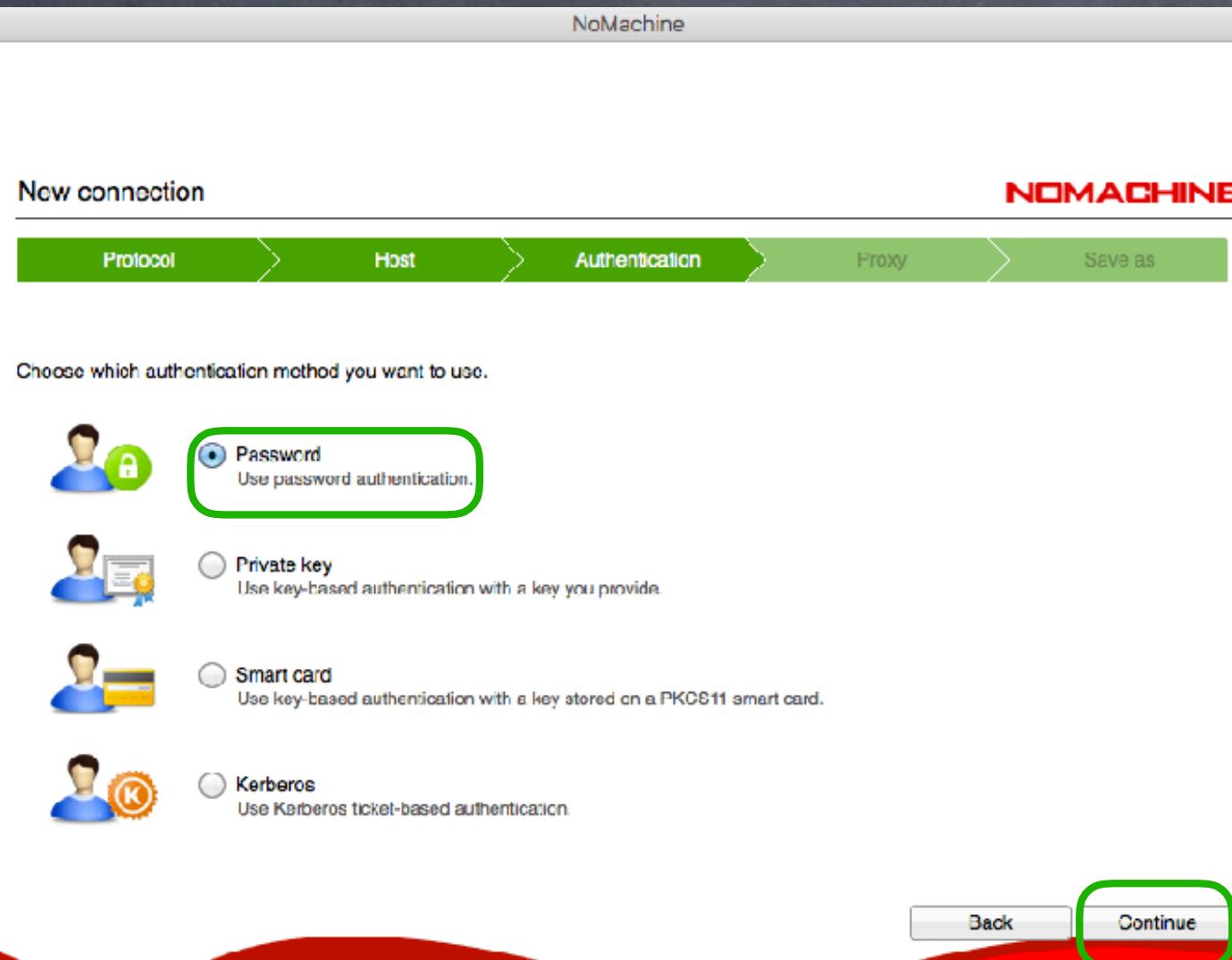
Use the system login  
This is the default. Choose this method to use your system password, key-based authentication or another authentication method supported by SSH.

Use the NoMachine login  
Use a server-specific RSA or DSA key and a password. Choose this method if the server is older than version 4 or if you need to use advanced features like guest logins.

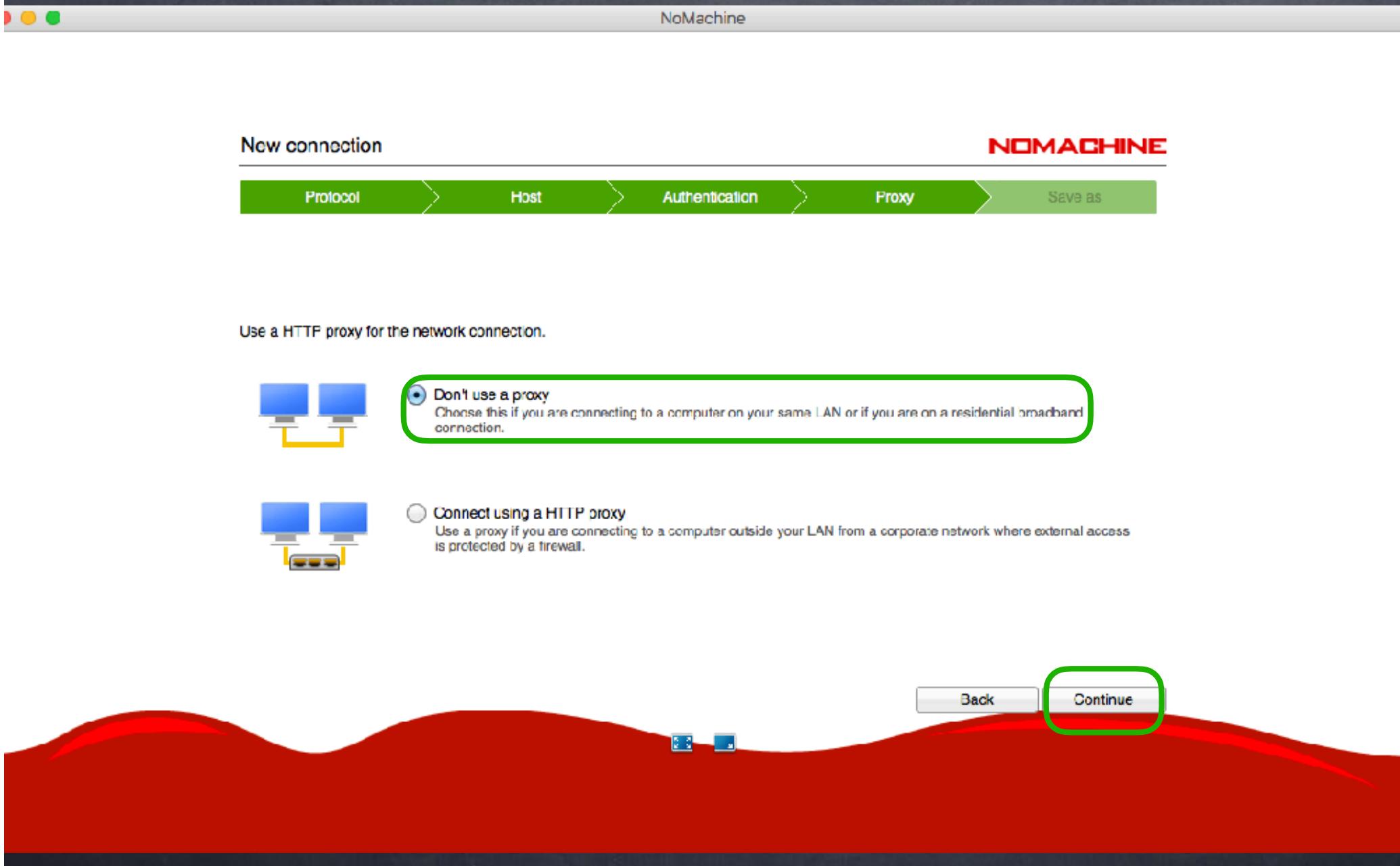
Back Continue

Apps on H2: intro R. D'Auria, Ph1

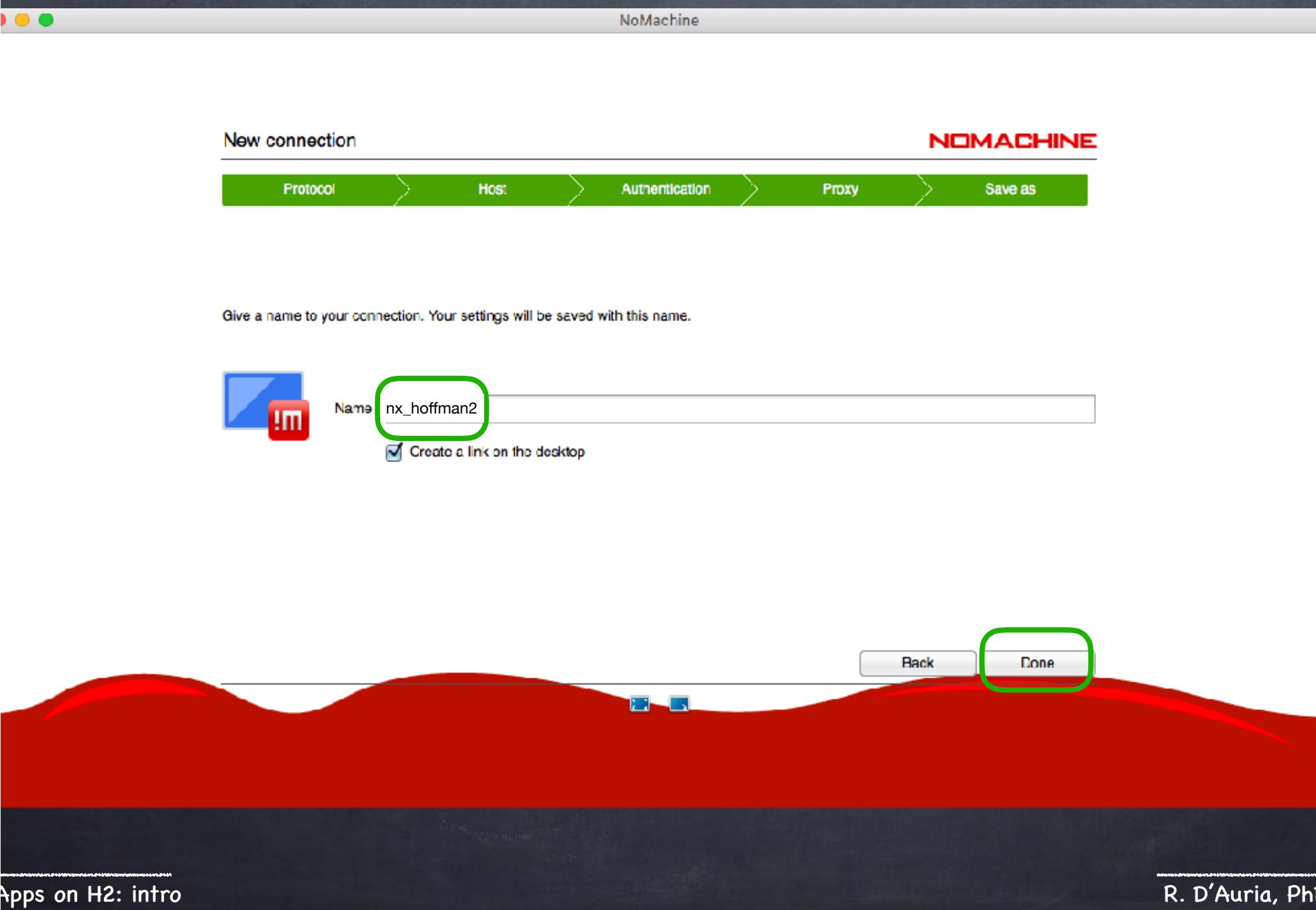
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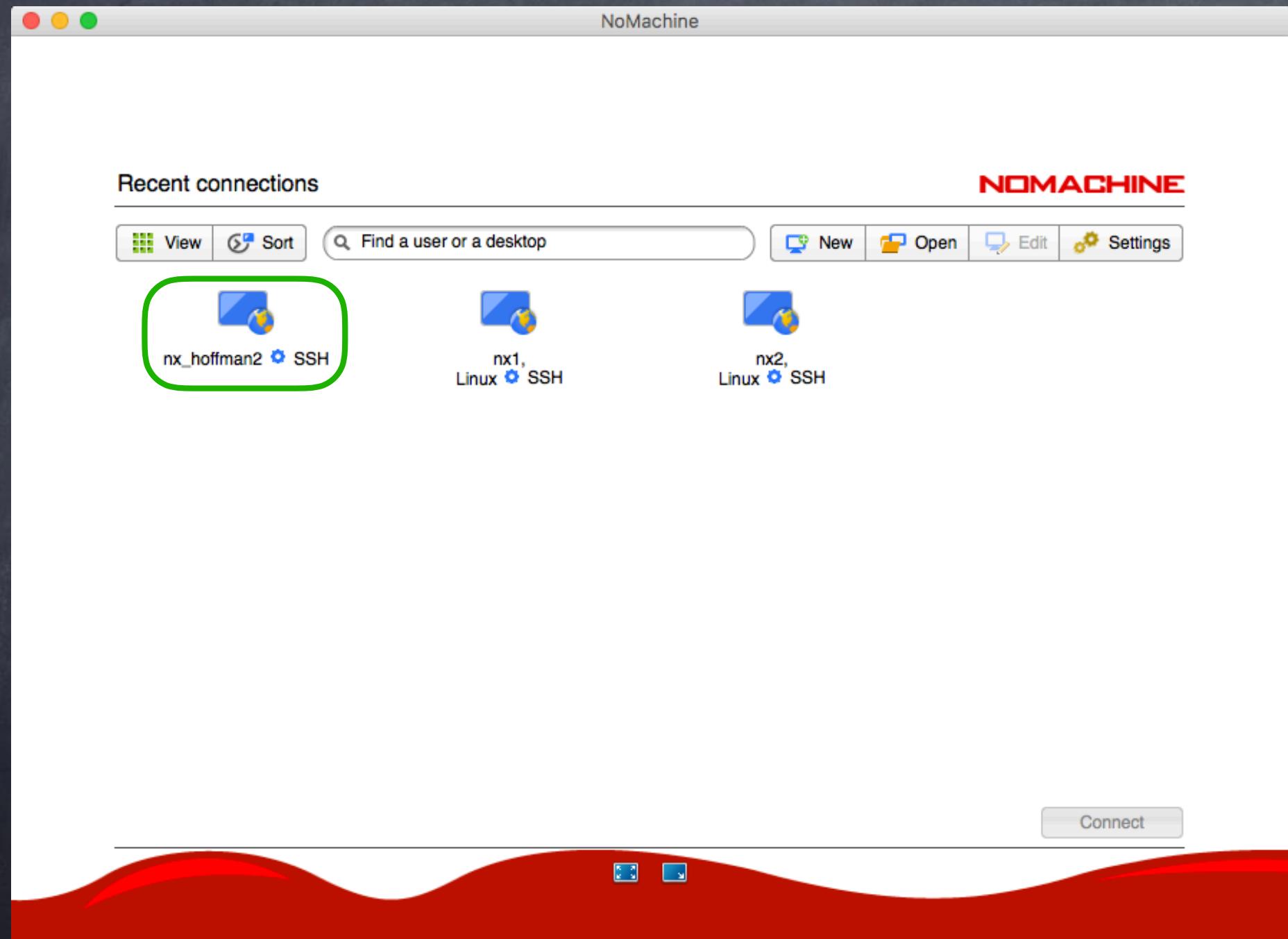
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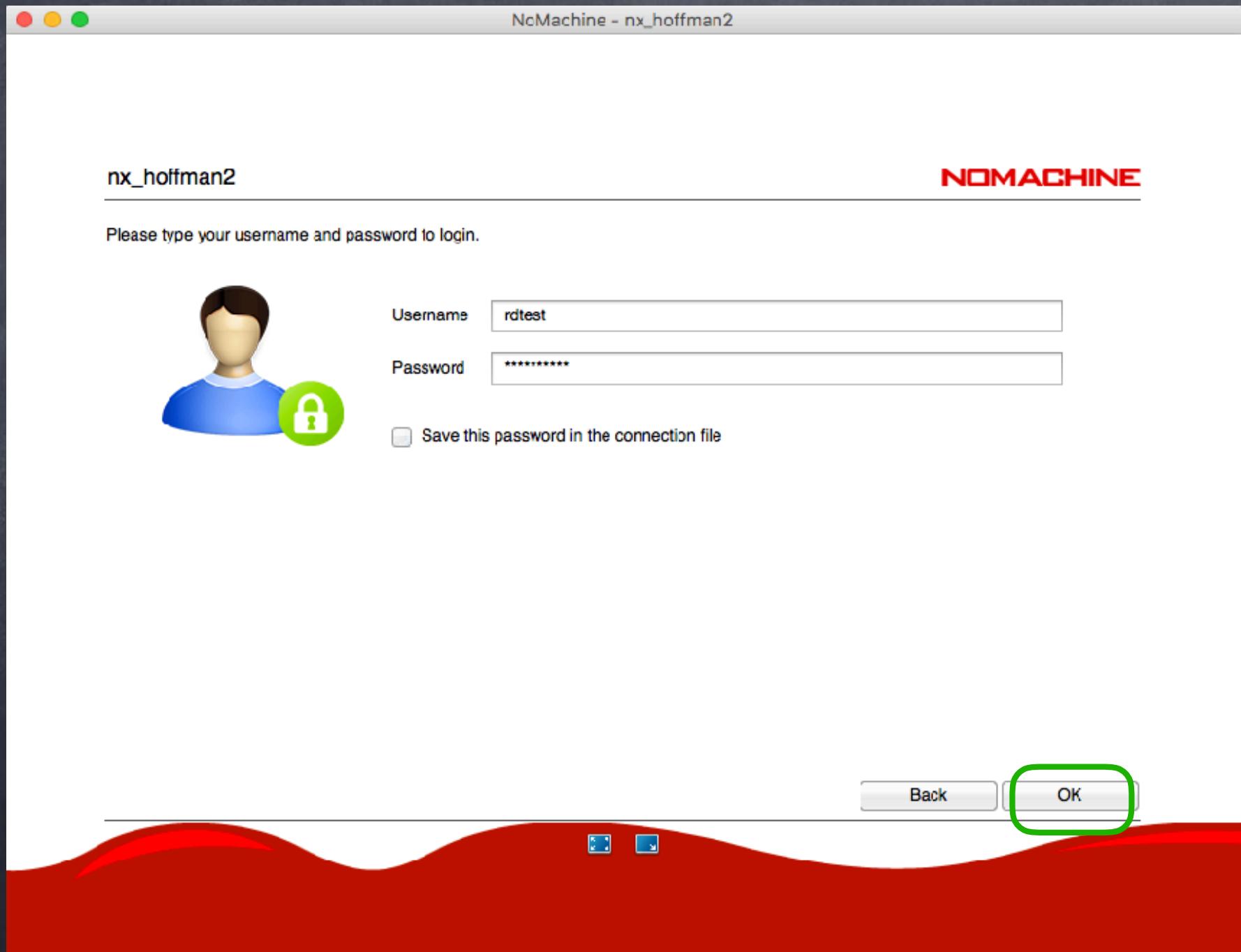
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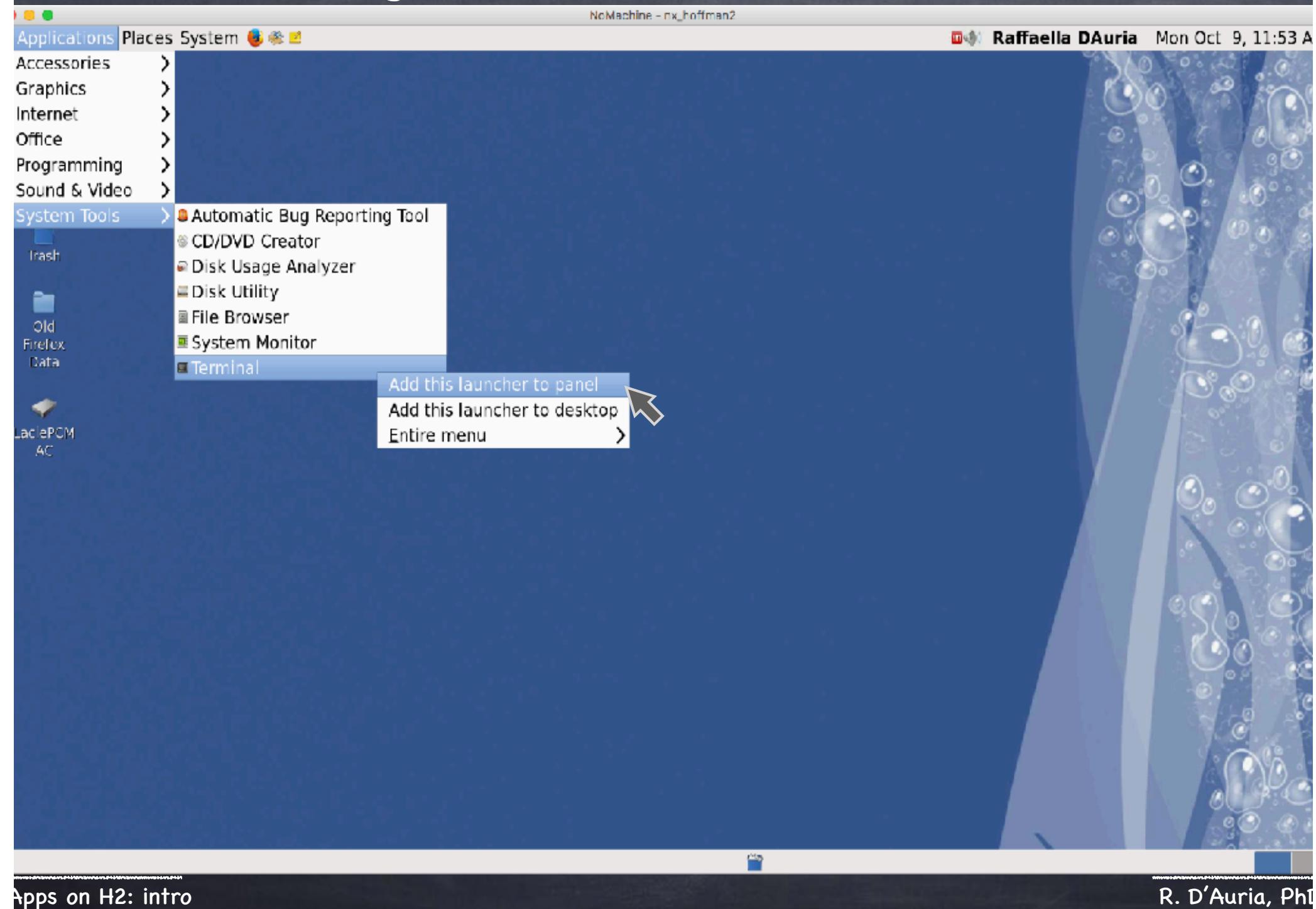
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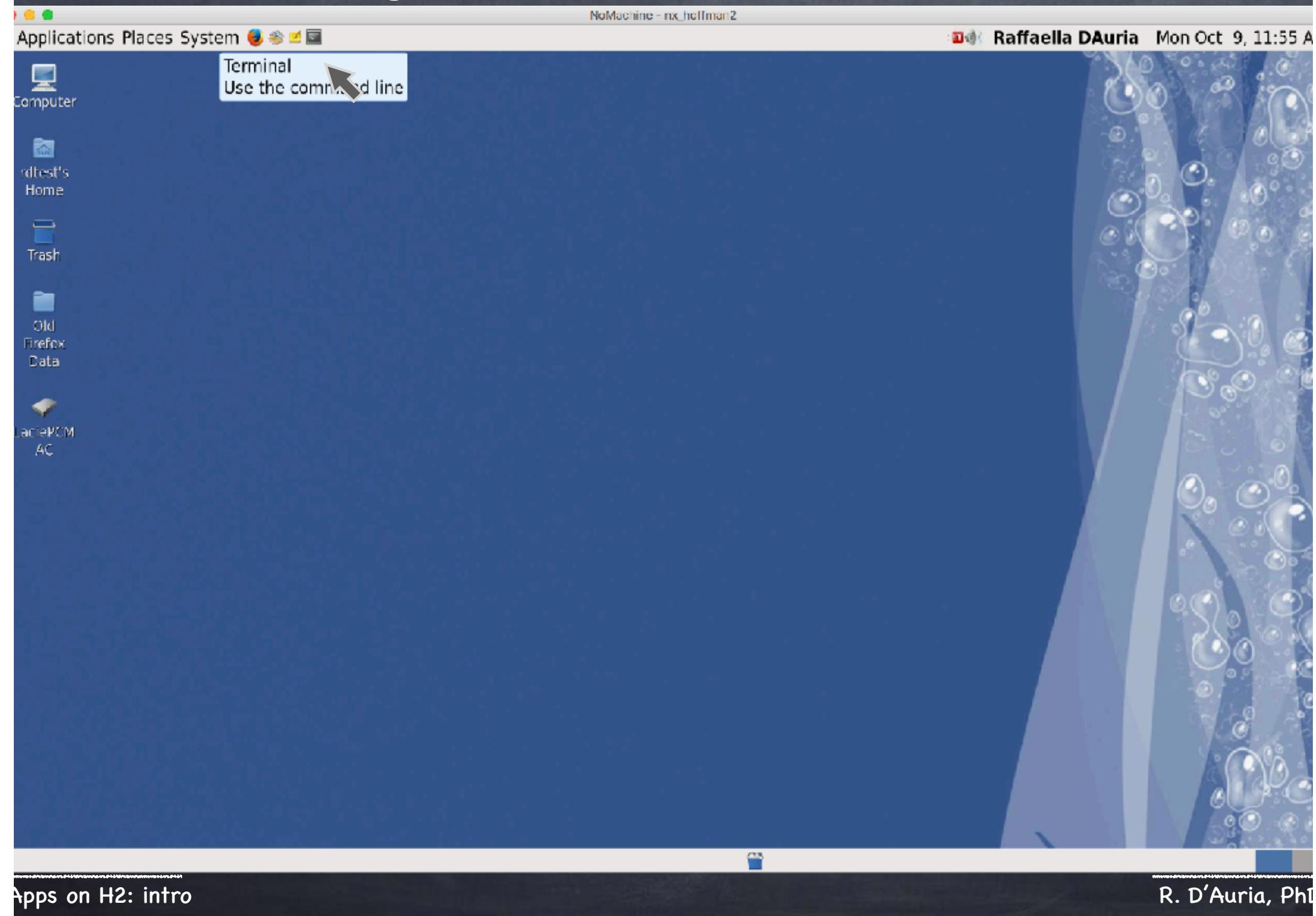
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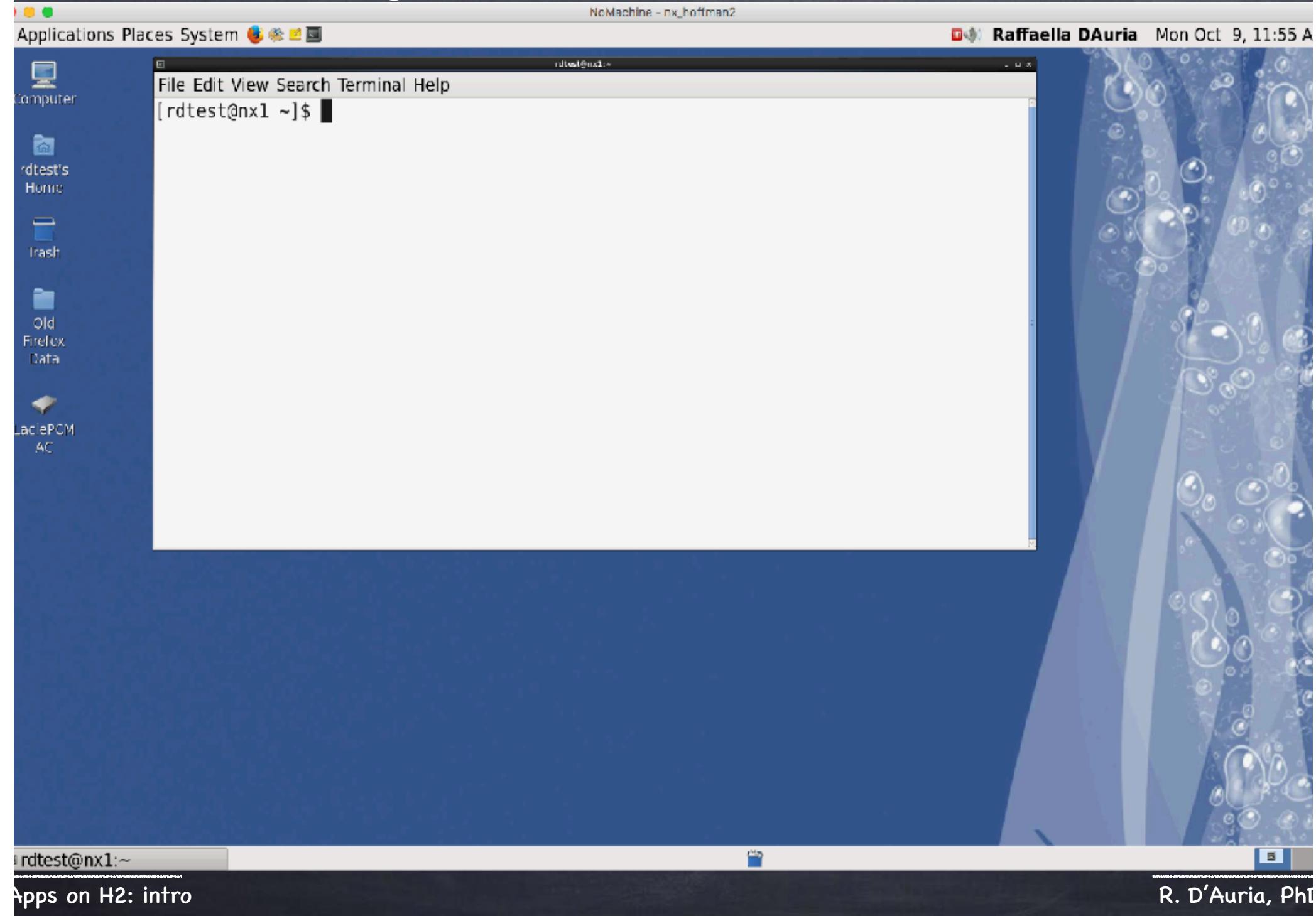
# Connecting to the Hoffman2 Cluster via NX



# Connecting to the Hoffman2 Cluster via NX



# Connecting to the Hoffman2 Cluster via NX



# Transferring your data/code on Hoffman2

The screenshot shows a web browser displaying the UCLA Hoffman2 Cluster User Guide. The URL in the address bar is <https://www.hoffman2.idre.ucla.edu>. The page features a navigation menu with tabs: ACCESS, COMPUTING, DATA STORAGE, FILE TRANSFER (which is circled in green), and SOFTWARE. A sidebar on the left contains links for About, User Support, FAQ, Getting started, News, Security policy, Status, How to acknowledge the Hoffman2 cluster program, and How to use this site. The main content area includes a search bar, a breadcrumb trail (You are here: Home), and sections for Recent Announcements, Free Classes, and Stata 15. The overall theme is dark blue and grey.

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**Stata 15** A new version of Stata has been installed. See [Stata 15 available](#) for further information.

# Transferring your data/code on Hoffman2

The screenshot shows a web browser window with the following details:

- Address Bar:** https://www.hoffman2.idre.ucla.edu/file-transfer/
- Page Title:** idre UCLA Hoffman2 Cluster User Guide
- Search Bar:** Search this website
- Report Errors:** Report Types and Errors
- Navigation Bar:** ACCESS, COMPUTING, DATA STORAGE, FILE TRANSFER (highlighted), SOFTWARE
- Left Sidebar (About):**
  - About
  - User Support
  - FAQ
  - Getting started
  - News
  - Security policy
  - Status
  - How to acknowledge the Hoffman2 cluster program
  - How to use this site
- Content Area:**
  - You are here: Home / File Transfer
  - ## File Transfer

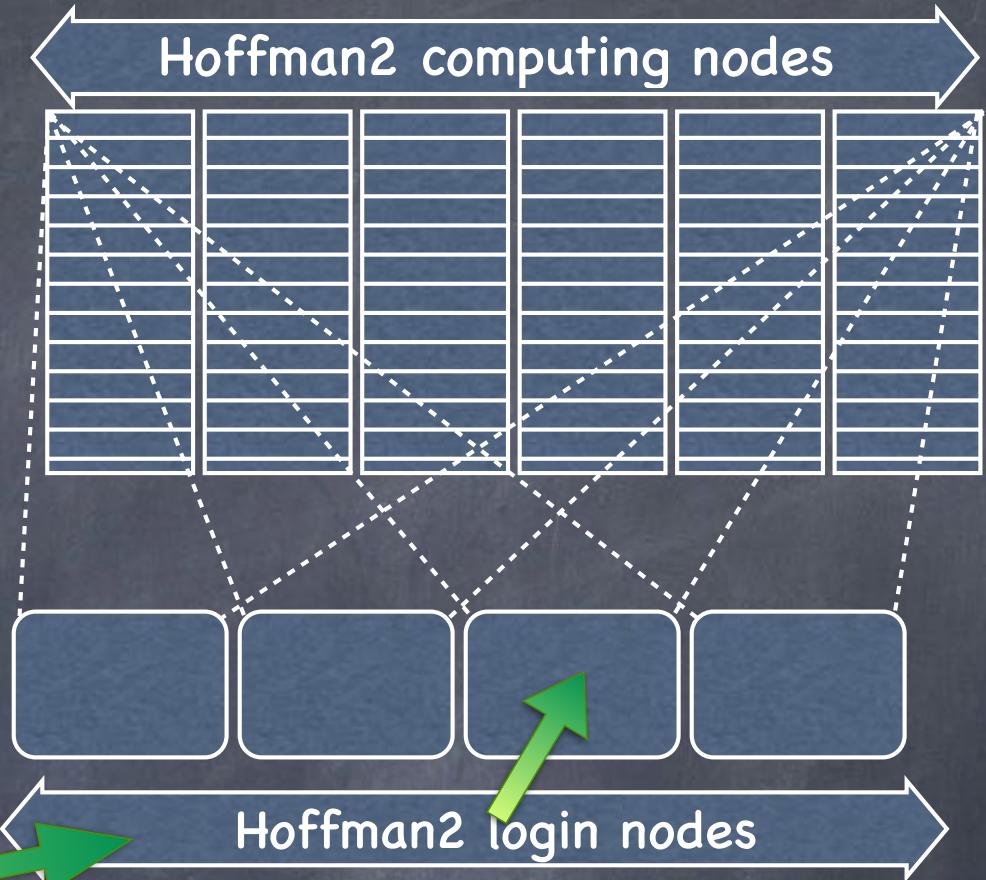
    - Contents [hide]**
    - Globus
    - scp and sftp
    - rsync
    - UCLA/UC Grid Portals (will retire soon)
  - ## Globus

Globus is a software tool to transfer files across the web in a reliable, high-performance and secure way. It provides fault-tolerant, fire-and-forget data transfer using simple web or command line interfaces. It is appropriate for transferring very large files either between your desktop machine and a remote machine like the Hoffman2 Cluster, or between two remote machines on which you have accounts; both remote machines need to be part of the Globus project. All XSEDE resources are configured as Globus endpoints.

See [High-speed file transfer with Globus](#) for information on using Globus.
  - ## scp and sftp

For security reasons, Hoffman2 Cluster allows file transfer only with scp or sftp or grid-ftp. For the same reason, you should use an scp or sftp client on your local machine. You should not use the scp command on the cluster.

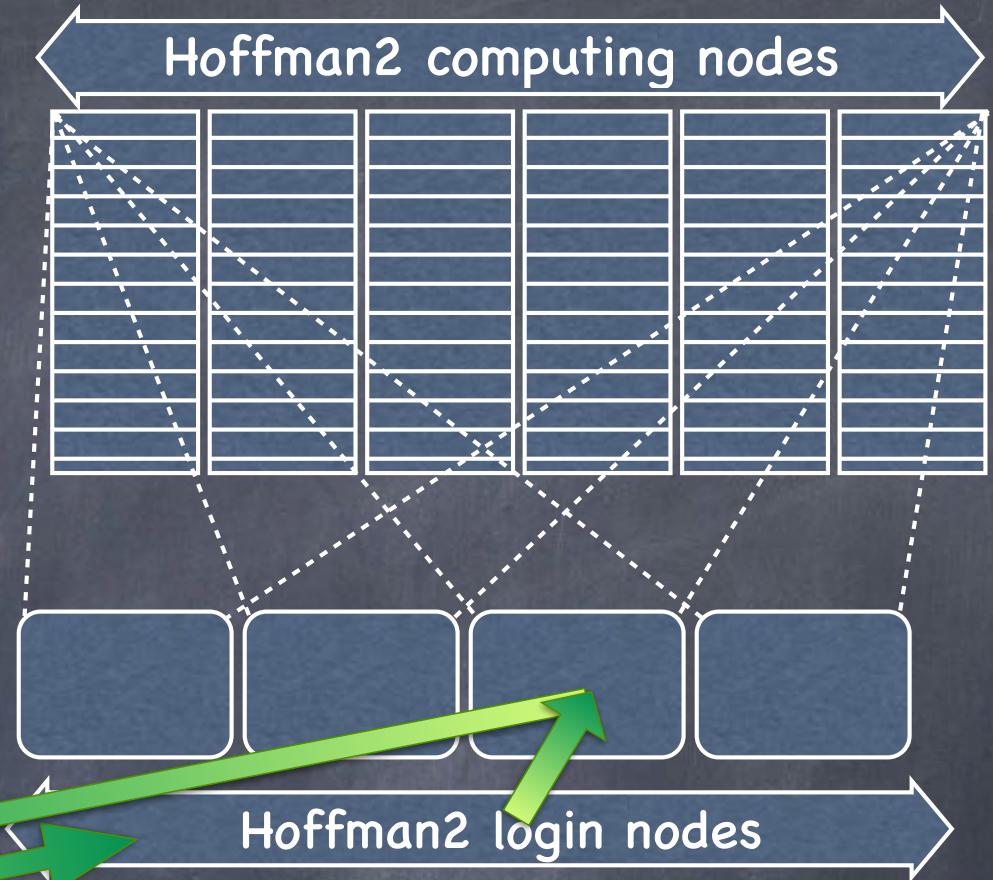
# Using the Hoffman2 cluster: How?



# Using the Hoffman2 cluster: How?



Hoffman2 user



Hoffman2 login nodes

# Using the Hoffman2 cluster: How?

## Unix command line

```
~ — rdtest@login1:~ — ssh -Y rdtest@hoffman2.idre.ucla.edu
Last login: Mon Oct  9 11:33:46 on ttys004
[dauria@alba:~> rdtest
[rdtest@hoffman2.idre.ucla.edu's password:
Warning: No xauth data; using fake authentication data for X11 forwarding.
Last login: Mon Oct  9 12:31:27 2017 from alba.ats.ucla.edu
Welcome to the Hoffman2 Cluster!

Hoffman2 Home Page:      http://www.hoffman2.idre.ucla.edu
Consulting:                https://support.idre.ucla.edu/helpdesk

All login nodes should be accessed via "hoffman2.idre.ucla.edu".

Please do NOT compute on the login nodes.

Processes running on the login nodes which seriously degrade others'
use of the system may be terminated without warning. Use qrsh to obtain
an interactive shell on a compute node for CPU or I/O intensive tasks.

The following news items are currently posted:

IDRE Fall 2017 HPC Classes
Stata 15 available
News Archive On Web Site

Enter shownews to read the full text of a news item.
[rdtest@login1 ~]$
```

**Now what?**

# Using the Hoffman2 cluster: How? Unix command line

The screenshot shows the homepage of the IDRE (Institute for Digital Research and Education) website at <https://idre.ucla.edu>. The page features a header with the IDRE logo, UCLA branding, and social media links. A navigation bar includes links for About, People, Research, News, and Events. The main content area has a large yellow "WHAT WE DO" section with a mission statement and a "MORE ABOUT US" button. To the right is an "UPCOMING EVENTS" section with three listed events and a "View All Events" link. A green oval highlights the browser's address bar showing the URL and another highlights the "View All Events" link.

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The IDRE mission is to support, advance and guide a campus-wide program to position UCLA as a world leader in research and education in computational thinking.

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### UPCOMING EVENTS

[Running Applications on Hoffman2 Cluster: An Introduction](#)  
October 10, 2017 @ 10:00 am - 12:00 pm

[Running Applications on Hoffman2 Cluster: Case Studies](#)  
October 12, 2017 @ 10:00 am - 12:00 pm

[Introduction to SPSS](#)  
October 16, 2017 @ 9:00 am - 12:00 pm

[View All Events](#)

# Using the Hoffman2 cluster: How? Unix command line



## Computing Environment on Linux – I

October 26, 2017 @ 2:00 pm - 4:00 pm

5628 Math Science Building, UCLA,

Part-I session of Computing Environment on Linux class is aimed to help researchers who are new to the Linux system. This two hour session will introduce basic Unix/Linux commands, shells, as well as a few editors available on most of the flavors of Linux operating system. The user should be able to log in to a Linux system and use it to do the normal tasks after going through this session.

[Find out more »](#)

---

Free

## Computing Environment on Linux – II

October 31, 2017 @ 2:00 pm - 4:00 pm

5628 Math Science Building, UCLA,

The second session is regarding the use of Linux system for computation. It will describe the compilation and execution procedures for a given source program. A sample software code will be used to demonstrate the computing tools such as `makefile`, `debugger`, and `profiler` which are available under most Linux environments.

[Find out more »](#)

# Using the Hoffman2 cluster: How?

## Unix command line, a couple of handy commands

- navigation:

- ◆ `ls`

- ◆ `ls -a`

- ◆ `ls -l`

- ◆ `ls -lat`

- ◆ `ls -latr`

- ◆ `cd $SCRATCH`

- ◆ `pwd`

- ◆ `mkdir $HOME/test; cd $HOME/test`

- ◆ `pwd`

# Using the Hoffman2 cluster: How?

## Unix command line, a few handy concepts

- environmental variables:
  - ♦ \$PATH
  - ♦ \$LD\_LIBRARY\_PATH
  - ♦ \$HOME
  - ♦ \$SCRATCH
- How to check the contents of an env var:
  - ♦ echo \$HOME

# Using the Hoffman2 cluster: How?

Unix command line, a few handy commands:

- just look at a file (no editing):
  - ◆ `less $HOME/.bashrc`
  - ◆ `cat $HOME/.bashrc`
- look to the first few lines of a file:
  - ◆ `head $HOME/.bashrc`
  - ◆ `head -n 5 $HOME/.bashrc`
- look to the last few lines of a file:
  - ◆ `tail $HOME/.bashrc`
  - ◆ `tail -n 5 $HOME/.bashrc`
- look to the last few lines of a file on the fly:
  - ◆ `tail -f /u/local/licenses/LOGS/logit.matlab`
  - ◆ Control-C (to exit)

# Using the Hoffman2 cluster: How?

## Unix command line, a couple of handy commands

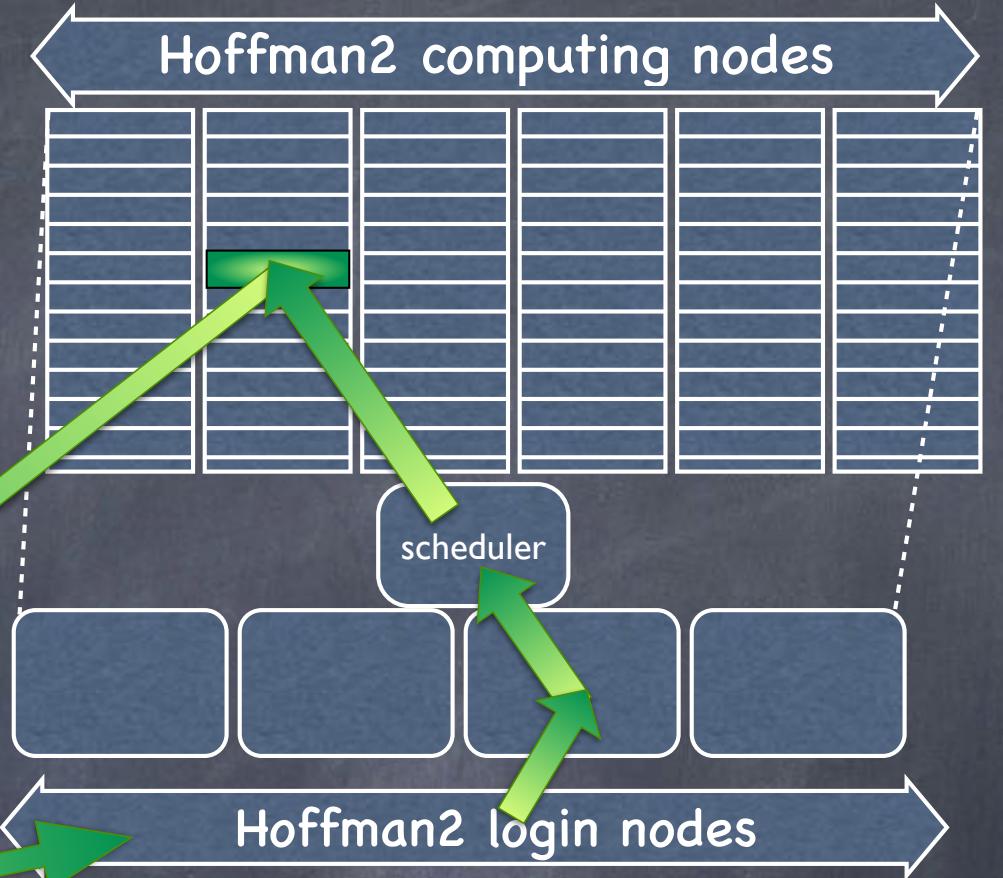
- editing w/out X11-forwarding enabled:
  - ◆ nano
  - ◆ emacs
  - ◆ vi
- editing w/ X11-forwarding enabled:
  - ◆ (nano)
  - ◆ gedit &
  - ◆ emacs &
  - ◆ gvim &

# Using the Hoffman2 cluster: starting an interactive session



```
[rdtest@login2 ~]$ qrsh -l h_rt=2:00:00,h_data=4g -pe shared 2  
[rdtest@n9860 ~]$
```

Hoffman2 user



Q?: Why is the command "qrsh" understood by the unix-shell?

A?: b/c it is in your \$PATH

# How to learn more about qrsh...

The screenshot shows a web browser displaying the UCLA Hoffman2 Cluster User Guide. The URL in the address bar is <https://www.hoffman2.idre.ucla.edu>. The page features a top navigation bar with icons for back, forward, search, and other functions. On the right side of the header is a link to "Report Typos and Errors". The main content area includes the UCLA idre logo, the title "UCLA Hoffman2 Cluster User Guide", a search bar labeled "Search this websi", and a navigation menu with tabs: ACCESS, COMPUTING (which is highlighted with a green oval), DATA STORAGE, FILE TRANSFER, and SOFTWARE. A sidebar on the left contains links to various resources: About, User Support, FAQ, Getting started, News, Security policy, Status, How to acknowledge the Hoffman2 cluster program, and How to use this site.

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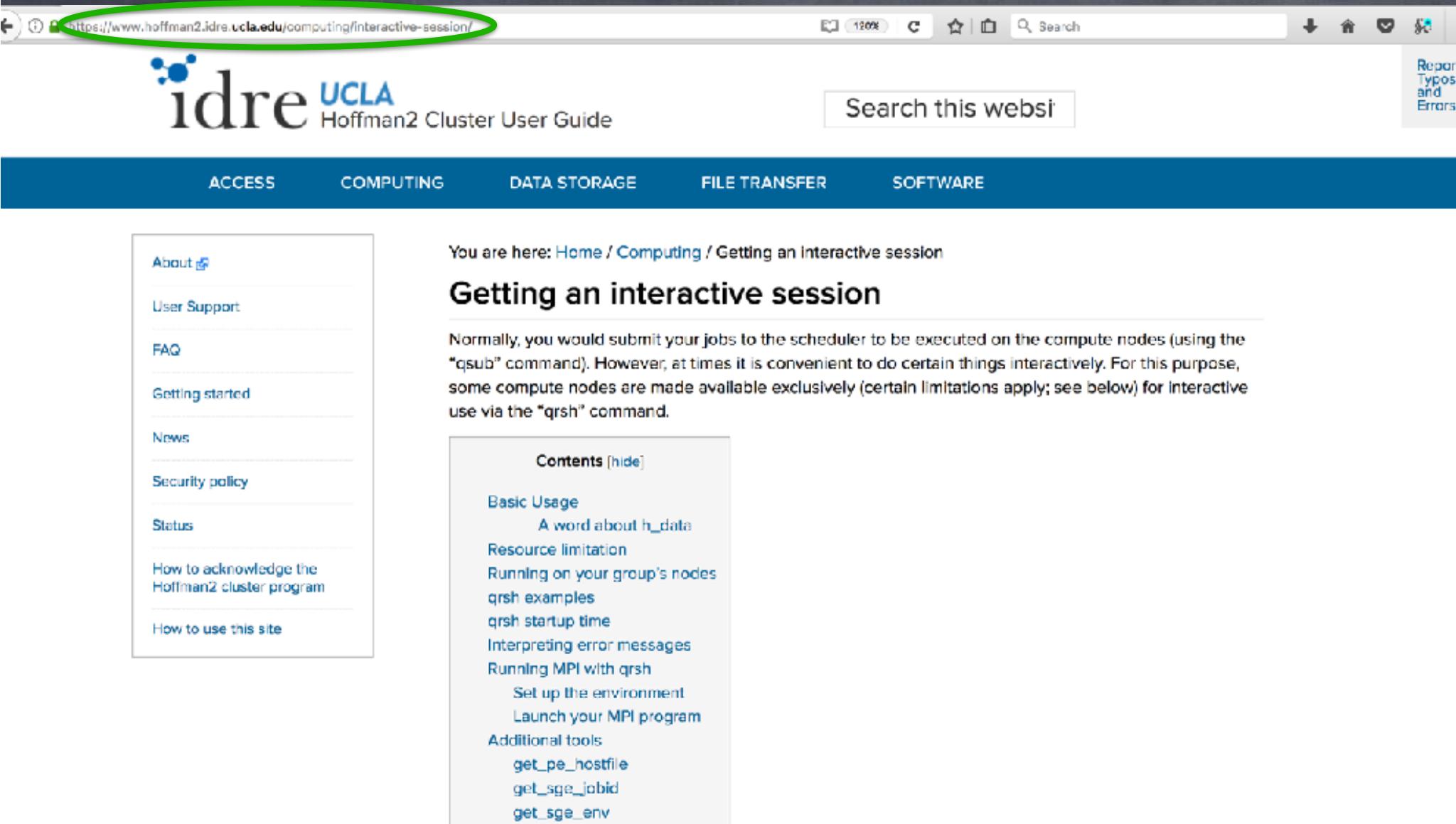
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**Stata 15** A new version of Stata has been installed. See [Stata 15 available](#) for further information.

# How to learn more about qrsh...

The screenshot shows a web browser window with the URL <https://www.hoffman2.idre.ucla.edu/computing/> highlighted by a green oval. The page title is "idre UCLA Hoffman2 Cluster User Guide". A search bar at the top right contains the placeholder "Search this website". Below the header, a navigation menu has "COMPUTING" selected, indicated by a blue background. The main content area shows the "Computing" page with a sidebar containing links like "About", "User Support", "FAQ", "Getting started", "News", "Security policy", "Status", "How to acknowledge the Hoffman2 cluster program", and "How to use this site". A "Contents [hide]" box lists "General information", "Interactive jobs", "Batch jobs", "GPU Computing", "Additional Information", and "How to ...". The "Interactive jobs" link is circled in green. The "General information" section includes a bullet point for "Job Queues and Policy". The "Interactive jobs" section includes a bullet point for "How to Get an Interactive Session", which is also circled in green. The "Batch Jobs" section includes bullet points for "Submitting a Job" and "Commonly-Used UGE Commands".

# How to learn more about qrsh...



The screenshot shows a web browser window with the following details:

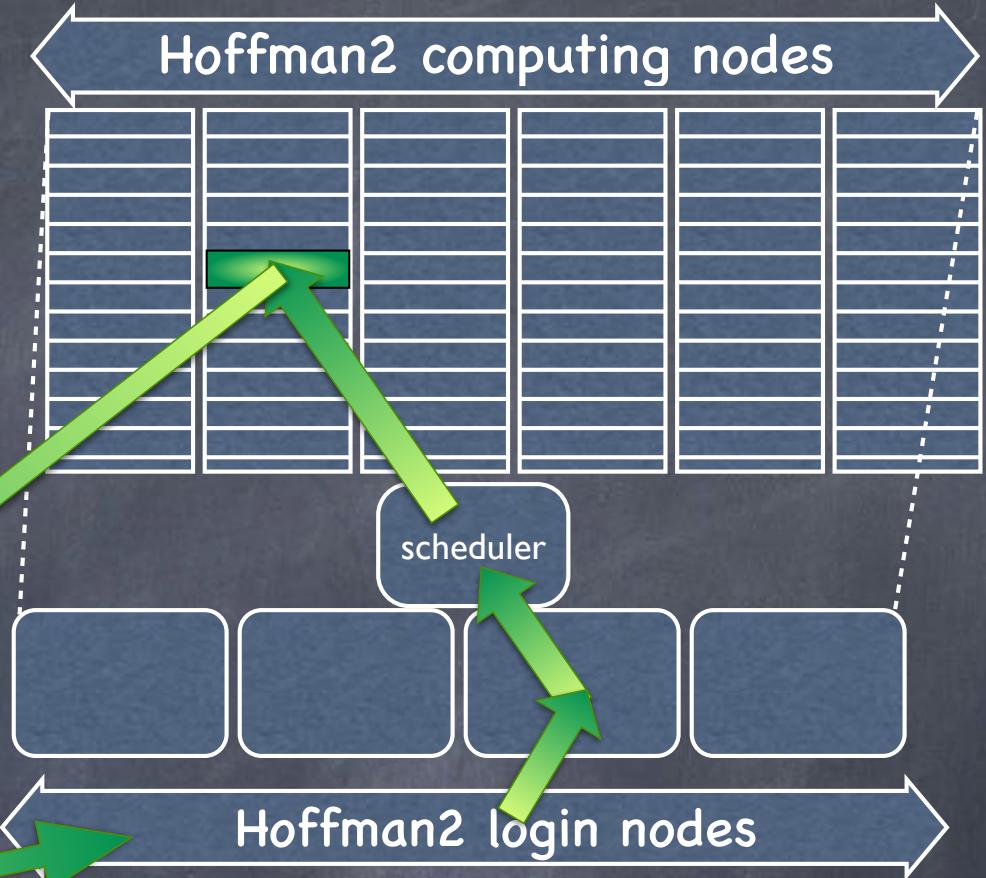
- Address Bar:** https://www.hoffman2.idre.ucla.edu/computing/interactive-session/ (highlighted with a green oval)
- Page Title:** idre UCLA Hoffman2 Cluster User Guide
- Search Bar:** Search this website
- Report Typos and Errors:** Link in the top right corner.
- Navigation Bar:** ACCESS, COMPUTING, DATA STORAGE, FILE TRANSFER, SOFTWARE
- Left Sidebar (About):**
  - About
  - User Support
  - FAQ
  - Getting started
  - News
  - Security policy
  - Status
  - How to acknowledge the Hoffman2 cluster program
  - How to use this site
- Current Location:** You are here: Home / Computing / Getting an interactive session
- Section Header:** Getting an interactive session
- Text Content:** Normally, you would submit your jobs to the scheduler to be executed on the compute nodes (using the "qsub" command). However, at times it is convenient to do certain things interactively. For this purpose, some compute nodes are made available exclusively (certain limitations apply; see below) for interactive use via the "qrsh" command.
- Table of Contents:**
  - Contents [hide]
  - Basic Usage
    - A word about h\_data
    - Resource limitation
    - Running on your group's nodes
    - qrsh examples
    - qrsh startup time
    - Interpreting error messages
    - Running MPI with qrsh
      - Set up the environment
      - Launch your MPI program
  - Additional tools
    - get\_pe\_hostfile
    - get\_sge\_jobid
    - get\_sge\_env

# Using the Hoffman2 cluster: starting an interactive application



```
[rdtest@login2 ~]$ qrsh -l h_rt=2:00:00,h_data=4g -pe shared 2  
[rdtest@login2 ~]$ module load matlab  
[rdtest@login2 ~]$ matlab &
```

Hoffman2 user



Side note: "module load <app>" places the <app> in your \$PATH

# How to learn more about environmental modules...

The screenshot shows a web browser displaying the UCLA Hoffman2 Cluster User Guide. The URL in the address bar is <https://www.hoffman2.idre.ucla.edu>. The page features a header with the idre logo, the UCLA logo, and a search bar labeled "Search this website". Below the header is a blue navigation bar with tabs: ACCESS, COMPUTING, DATA STORAGE, FILE TRANSFER, and SOFTWARE, with SOFTWARE circled in green. The main content area includes a sidebar with links like About, User Support, FAQ, Getting started, News, Security policy, Status, How to acknowledge the Hoffman2 cluster program, and How to use this site. The main content section is titled "Home" and welcomes visitors to the Hoffman2 Cluster User Guide, encouraging them to click on navigation tabs or sidebar items for usage information. It also highlights "Free Classes" and "Stata 15" announcements.

https://www.hoffman2.idre.ucla.edu

Report Typos and Errors

idre

UCLA

Hoffman2 Cluster User Guide

Search this website

ACCESS COMPUTING DATA STORAGE FILE TRANSFER SOFTWARE

About

User Support

FAQ

Getting started

News

Security policy

Status

How to acknowledge the Hoffman2 cluster program

How to use this site

You are here: Home

## Home

Welcome to the Hoffman2 Cluster User Guide. To look up usage information, click on one of the navigation tabs above or the sidebar items on the left.

### Recent Announcements

**Free Classes** IDRE Research Technology Group is pleased to present Fall Quarter classes. There is no charge or fee to attend these classes. See [IDRE Fall 2017 HPC Classes](#)

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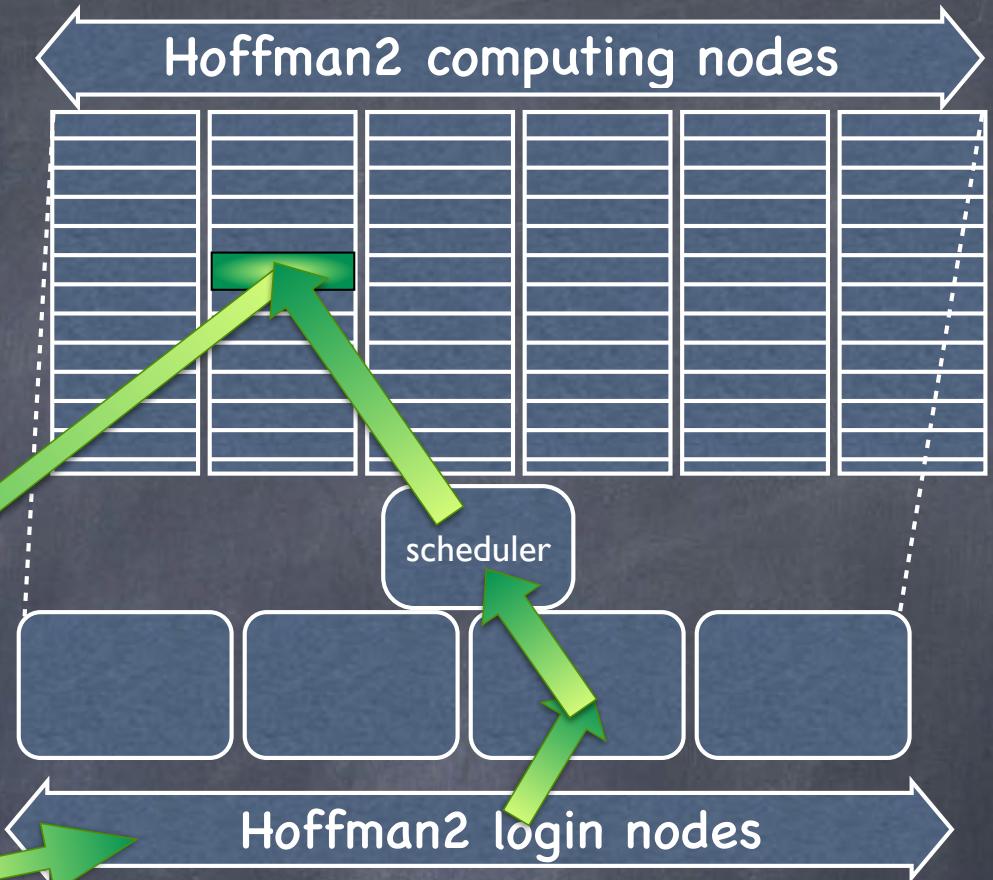
- Address Bar:** https://www.hoffman2.idre.ucla.edu/software/ (highlighted with a green oval)
- Toolbar:** Back, Forward, Stop, Refresh, 120%, Home, Search, Download, etc.
- Header:** idre (with a blue logo), UCLA, Hoffman2 Cluster User Guide, Report Typos and Errors
- Search:** Search this website
- Navigation Bar:** ACCESS, COMPUTING, DATA STORAGE, FILE TRANSFER, SOFTWARE (the SOFTWARE tab is selected)
- Left Sidebar:** About, User Support, FAQ, Getting started, News, Security policy, Status, How to acknowledge the Hoffman2 cluster program, How to use this site
- Current Page Content:** You are here: Home / Software
- Section Header:** Software
- Text:** This page provides a summary of most of the software available on the Hoffman2 cluster
- Contents:** Compilers, Editors, Environmental Modules (highlighted with a green oval), Installations requests, Applications Packages
  - Bioinformatics and Biostatistics
  - Chemistry and Chemical Engineering
  - Engineering and Mathematics
  - Statistics
  - Visualization

# How to learn more about environmental modules...

The screenshot shows a web browser window with the following details:

- Address Bar:** https://www.hoffman2.idre.ucla.edu/computing/modules/ (The URL is circled in green).
- Toolbar:** Includes icons for back, forward, search, and other browser functions.
- Header:** The page is titled "UCLA Hoffman2 Cluster User Guide".
- Search:** A search bar with the placeholder "Search this website".
- Navigation:** A blue navigation bar with links: ACCESS, COMPUTING, DATA STORAGE, FILE TRANSFER, and SOFTWARE.
- Left Sidebar:** A sidebar with links: About, User Support, FAQ, Getting started, News, Security policy, Status, How to acknowledge the Hoffman2 cluster program, and How to use this site.
- Content Area:** The main content is titled "modules". It describes environmental modules as a utility for modifying shell environment variables. It includes a "Contents [hide]" section with links to various sub-topics: Basic commands, module command in interactive sessions, module command in scripts for batch execution, module command in scripts for batch execution of serial jobs, module command in scripts for batch execution of parallel jobs, module command in scripts for batch execution of parallel jobs using shared memory, module command in scripts for batch execution of parallel jobs using IntelMPI library, and module command in scripts for batch execution of parallel jobs using IntelMPI library and.
- Footer:** The footer contains the text "Apps on H2: intro" and "R. D'Auria, PhD".

# Using the Hoffman2 cluster: running Matlab



What applications are  
available on the  
Hoffman2 cluster?

# Applications already available on Hoffman2

The screenshot shows a web browser displaying the UCLA Hoffman2 Cluster User Guide. The URL in the address bar is <https://www.hoffman2.idre.ucla.edu>. The page features a header with the idre logo, the UCLA logo, and a search bar labeled "Search this website". Below the header is a navigation bar with tabs: ACCESS, COMPUTING, DATA STORAGE, FILE TRANSFER, and SOFTWARE, with SOFTWARE circled in green. On the left, there is a sidebar with links: About, User Support, FAQ, Getting started, News, Security policy, Status, How to acknowledge the Hoffman2 cluster program, and How to use this site. The main content area is titled "Home" and includes sections for Recent Announcements, Free Classes, and Stata 15.

Report Typos and Errors

UCLA  
Hoffman2 Cluster User Guide

Search this website

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How to acknowledge the Hoffman2 cluster program

How to use this site

You are here: [Home](#)

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# Applications already available on Hoffman2

The screenshot shows a web browser displaying the "Software" page of the Hoffman2 Cluster User Guide. The URL in the address bar is <https://www.hoffman2.idre.ucla.edu/software/>. A green circle highlights the URL.

The page features the UCLA IDRE logo at the top left, a search bar at the top right, and a navigation menu with tabs for ACCESS, COMPUTING, DATA STORAGE, FILE TRANSFER, and SOFTWARE (which is currently selected).

The main content area includes a sidebar with links to About, User Support, FAQ, Getting started, News, Security policy, Status, How to acknowledge the Hoffman2 cluster program, and How to use this site. The main content area displays the "Software" section, which provides a summary of available software and lists various categories and sub-categories.

**Software Categories:**

- Contents [hide]
- Compilers
- Editors
- Environmental Modules
- Installations requests
- Applications Packages
  - Bioinformatics and Biostatistics
  - Chemistry and Chemical Engineering
  - Engineering and Mathematics
  - Statistics
  - Visualization
  - Languages and Debuggers
  - Integrated development environments (IDEs)
  - Programming Libraries
  - Misellaneous

# Applications already available on Hoffman2

```
[rdtest@login2 ~]$ module av
```

----- /u/local/Modules/modulefiles -----

ATS	gcc/4.4(default)	netcdf/4.1.3(default)
R/2.12.0	gcc/4.7.2	netcdf/4.1.3-shared
R/2.12.1	gcc/4.9.3	netcdf/4.1.3_i
R/2.12.2	gcc/6.3.0	netcdf/4.2.3-c
R/2.13.2	gcta/0.93.9	netcdf/4.4.2-fortran
R/2.15.1	gdal/1.9.2(default)	ngsplot/2.47
R/2.9.1	gdal/2.2.0	nwchem/6.5(default)
R/3.0.1	gdc/0.30	octave/3.6.1
R/3.1.1	gdc/4.9.3(default)	octave/3.6.4(default)
R/3.2.1	geant4/10.00.p02_wGDML	oommf/12b0
R/3.2.3(default)	geant4/4.9.3.p02(default)	openbabel/2.3.1(default)
R/3.3.0	geant4/4.9.4.p02	openblas/0.2.18(default)
R/3.3.3	geant4/4.9.5	openblas/0.2.18-threaded
R/3.4.0	geant4/9.6.2	opencv/2.4.11
R/3.4.1	geant4/9.6.p02_wGDML	openmpi/1.6_gcc-4.4
Rstudio/0.98(default)	geos/3.4.2(default)	opensees/2.4.1

...

...

...

& many more...

# Applications already available on Hoffman2

```
[rdtest@login2 ~]$ module av python
```

```
----- /u/local/Modules/modulefiles -----
python/2.6(default) python/2.7.13      python/2.7.3      python/3.4      python/3.6.1_shared
python/2.7          python/2.7.13_shared python/3.1       python/3.6.1
```

```
[rdtest@login2 ~]$ module av matlab
```

```
----- /u/local/Modules/modulefiles -----
matlab/7.11        matlab/7.7        matlab/8.4        matlab/9.1
matlab/7.14        matlab/8.2        matlab/8.6(default) matlab/9.1_MCR
```

```
[rdtest@login2 ~]$ module av R
```

```
----- /u/local/Modules/modulefiles -----
R/2.12.0          R/2.13.2        R/3.0.1        R/3.2.3(default)   R/3.4.0
R/2.12.1          R/2.15.1        R/3.1.1        R/3.3.0          R/3.4.1
R/2.12.2          R/2.9.1        R/3.2.1        R/3.3.3          Rstudio/0.98(default)
```

```
[rdtest@login2 ~]$ module av intel
```

```
----- /u/local/Modules/modulefiles -----
intel/11.1         intel/12.1       intel/13.cs(default) intel/16.0.2      intelmpi/4.1.1    intelmpi/5.0.0
intel/12.0         intel/13.0       intel/14.cs        intel/17.0.1      intelmpi/4.1.3
```

# Applications already available on Hoffman2

```
[rdtest@login2 ~]$ module av python
----- /u/local/Modules/modulefiles -----
python/2.6(default) python/2.7.13      python/2.7.3      python/3.4      python/3.6.1_shared
python/2.7          python/2.7.13_shared  python/3.1       python/3.6.1
```

```
[rdtest@login2 ~]$ which python
/usr/bin/python
```

```
[rdtest@login2 ~]$ module load python/2.7.13_shared
```

The 'gcc/4.9.3' module is being loaded

These modules were already loaded: ATS intel/17.0.1

```
[rdtest@login2 ~]$ which python
/u/local/apps/python/2.7.13-shared/bin/python
```

```
[rdtest@login2 ~]$ python
Python 2.7.13 (default, Jul 28 2017, 10:36:35)
[GCC 4.9.3] on linux2
Type "help", "copyright", "credits" or "license" for more information.
>>>
```

# Applications already available on Hoffman2: Which python packages?

```
[rdtest@n9860 ~]$ module load python/2.7.13_shared
[rdtest@n9860 ~]$ pip freeze
Cython==0.26
virtualenv==15.1.0
[rdtest@n9860 ~]$ ls $HOME/.local
ls: cannot access /u/home/r/rdtest/.local: No such file or directory
[rdtest@n9860 ~]$ pip install numpy --user
Collecting numpy
  Downloading numpy-1.13.3-cp27-cp27m-manylinux1_x86_64.whl (16.6MB)
    100% |████████████████████████████████| 16.7MB
 46kB/s

Installing collected packages: numpy
Successfully installed numpy-1.13.3
[rdtest@n9860 ~]$ ls $HOME/.local/
bin  lib
[rdtest@n9859 ~]$ $HOME/.local/lib/python2.7/site-packages
numpy  numpy-1.13.3.dist-info
```

Some examples will be addressed in Thursday's class

# Applications already available on Hoffman2: Python

- Any python package installed with:
  - pip install —user
- Is installed in:
  - `$HOME/.local`
- most python packages install only libraries in:
  - `$HOME/.local/lib/python2.7/site-packages`
  - this location is automatically searched by python
  - this location is unique per python version
- some python packages install executables in:
  - `$HOME/.local/bin`
  - this location needs to be added to your `$PATH`
  - this location is not unique across different python versions

# Applications already available on Hoffman2: Python

```
[rdtest@n9860 ~]$ ls $HOME/.local/bin
```

```
f2py
```

```
[rdtest@n9859 ~]$ pip install misopy --user
```

```
[...]
```

```
Successfully installed backports.functools-lru-cache-1.4 cycler-0.10.0 matplotlib-2.1.0
misopy-0.5.4 pyparsing-2.2.0 pysam-0.12.0.1 python-dateutil-2.6.1 pytz-2017.2
scipy-0.19.1 six-1.11.0 subprocess32-3.2.7
```

```
[rdtest@n9860 ~]$ ls -t $HOME/.local/bin
```

```
run_miso.py  compare_miso  summarize_miso  exon_utils  sam_to_bam      miso
filter_events  miso_zip       plot.py        pe_utils     index_gff      f2py
test_miso      run_events_analysis.py  sashimi_plot   miso_pack    module_availability
```

```
[rdtest@n9860 ~]$ which miso
```

```
miso.py: Command not found.
```

```
[rdtest@login3 ~]$ echo " export PATH=$HOME/.local/bin:$PATH" >> $HOME/.bash_profile
```

```
[rdtest@login3 ~]$ tail -n1 $HOME/.bash_profile
```

```
export PATH=/u/home/r/rdtest/.local/bin
```

```
[rdtest@login3 ~]$ . /u/home/r/rdtest/.bash_profile
```

```
[rdtest@login3 ~]$ which miso.py
```

```
~/.local/bin/miso
```

# Applications already available on Hoffman2: Python

```
[rdtest@n9860 ~]$ head -n2 $HOME/.local/bin/miso  
#!/u/local/apps/python/2.7.13-shared/bin/python
```

```
[rdtest@n9860 ~]$
```

What happens when you have installed miso under more than one python version?

-> A cleaner alternative is to use python environments <-

```
[rdtest@n9860 ~]$ module load python/2.7.13_shared
```

```
[rdtest@n9860 ~]$ mkdir $HOME/mypython_env
```

```
[rdtest@n9860 ~]$ virtualenv env_python2.7.13
```

New python executable in /u/home/r/rdtest/mypython\_env/env\_python2.7.13/bin/python

Installing setuptools, pip, wheel...done.

```
[rdtest@n9860 ~]$ source env_python2.7.13/bin/activate
```

```
[env_python2.7.13] [rdtest@n9859 ~/mypython_env]$ which python
```

```
/u/home/r/rdtest/mypython_env/env_python2.7.13/bin/python
```

```
[env_python2.7.13] [rdtest@n9859 ~/mypython_env]$ pip install numpy
```

# Applications already available on Hoffman2: Which R packages?

```
[rdtest@n9860 ~]$ module load R/3.4.1
```

[...]

```
[rdtest@n9860 ~]$ R
```

```
R version 3.4.1 (2017-06-30) -- "Single Candle"
```

```
Copyright (C) 2017 The R Foundation for Statistical Computing
```

```
Platform: x86_64-pc-linux-gnu (64-bit)
```

[...]

```
Type 'q()' to quit R.
```

```
> library()
```

```
Packages in library '/u/home/r/rdtest/R/x86_64-pc-linux-gnu-library/3.4':
```

**bbmle**

**BH**

**Biobase**

Tools for General Maximum Likelihood Estimation

Boost C++ Header Files

Biobase: Base functions for Bioconductor

... & more...

# Applications already available on Hoffman2: Which R packages?

```
[rdtest@n9860 ~]$ module load R/3.4.1
```

```
[rdtest@n9860 ~]$ R
```

```
R version 3.4.1 (2017-06-30) -- "Single Candle"
```

```
Copyright (C) 2017 The R Foundation for Statistical Computing
```

```
Platform: x86_64-pc-linux-gnu (64-bit)
```

```
[...]
```

```
Type 'q()' to quit R.
```

```
> install.packages("xlsx", dependencies = TRUE)
```

```
Installing package into '/u/home/r/rdtest/R/x86_64-pc-linux-gnu-library/3.4'
```

```
(as 'lib' is unspecified)
```

```
--- Please select a CRAN mirror for use in this session --
```

```
[...]
```

```
** testing if installed package can be loaded
```

```
* DONE (xlsx)
```

# Running a batch job

Why?

# Running a batch job

The screenshot shows a web browser window with the following details:

- Address Bar:** https://www.hoffman2.idre.ucla.edu
- Toolbar:** Includes back, forward, search, and other standard browser icons.
- Header:** The page is titled "UCLA Hoffman2 Cluster User Guide".
- Header Buttons:** A blue "Report Typos and Errors" button is located in the top right corner.
- Navigation Tabs:** A horizontal menu bar with tabs: ACCESS, COMPUTING (which is circled in green), DATA STORAGE, FILE TRANSFER, and SOFTWARE.
- Search Bar:** A search input field with placeholder text "Search this website".
- Sidebar:** A vertical sidebar on the left containing links: About, User Support, FAQ, Getting started, News, Security policy, Status, How to acknowledge the Hoffman2 cluster program, and How to use this site.
- Main Content:** The main content area displays the "Home" page. It includes a breadcrumb trail ("You are here: Home"), the title "Home", a welcome message, and sections for "Recent Announcements" (Free Classes, Stata 15).

# Running a batch job

The screenshot shows a web browser displaying the [idre UCLA Hoffman2 Cluster User Guide](https://www.hoffman2.idre.ucla.edu/computing/). The URL is highlighted with a green oval at the top left. The page has a dark blue header with navigation links: ACCESS, COMPUTING (which is active), DATA STORAGE, FILE TRANSFER, and SOFTWARE. A search bar on the right says "Search this website". The main content area is titled "Computing". On the left, there's a sidebar with links like About, User Support, FAQ, Getting started, News, Security policy, Status, How to acknowledge the Hoffman2 cluster program, and How to use this site. The main content area shows a "Contents [hide]" box with links to General information, Interactive jobs, Batch Jobs (which is circled in green), GPU Computing, Additional Information, and How to ... . Below this, sections for General information, Interactive jobs, and Batch Jobs are listed with their own sub-links.

https://www.hoffman2.idre.ucla.edu/computing/ 100% C Search Report Typos and Errors

**idre** UCLA Hoffman2 Cluster User Guide

Search this website

ACCESS COMPUTING DATA STORAGE FILE TRANSFER SOFTWARE

About User Support FAQ Getting started News Security policy Status How to acknowledge the Hoffman2 cluster program How to use this site

You are here: Home / Computing

## Computing

Contents [hide]

- General information
- Interactive jobs
- Batch Jobs
- GPU Computing
- Additional Information
- How to ...

### General information

- [Job Queues and Policy](#)

### Interactive jobs

- [How to Get an Interactive Session](#)

### Batch Jobs

- [Submitting a Job](#)
- [Commonly-Used UGE Commands](#)

Apps on H2: intro R. D'Auria, Ph

# Running a batch job

```
#!/bin/bash
#$ -cwd
# error = Merged with joblog
#$ -o joblog.$JOB_ID
#$ -j y
#$ -l h_rt=1:00:00,h_data=1g
# Email address to notify
#$ -M $USER@mail
# Notify when
#$ -m bea

# echo job info on joblog:
echo "Job $JOB_ID started on:    `hostname -s`"
echo "Job $JOB_ID started on:    `date`"
echo " "

# load the job environment:
. /u/local/Modules/default/init/modules.sh
module load <APP>
module li
echo " "

# run <APP>
echo '<execution command>'<execution command>

# echo job info on joblog:
echo "Job $JOB_ID ended on:    `hostname -s`"
echo "Job $JOB_ID ended on:    `date`"
echo " "
```