Introduction to scientific computing

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Lecture overview

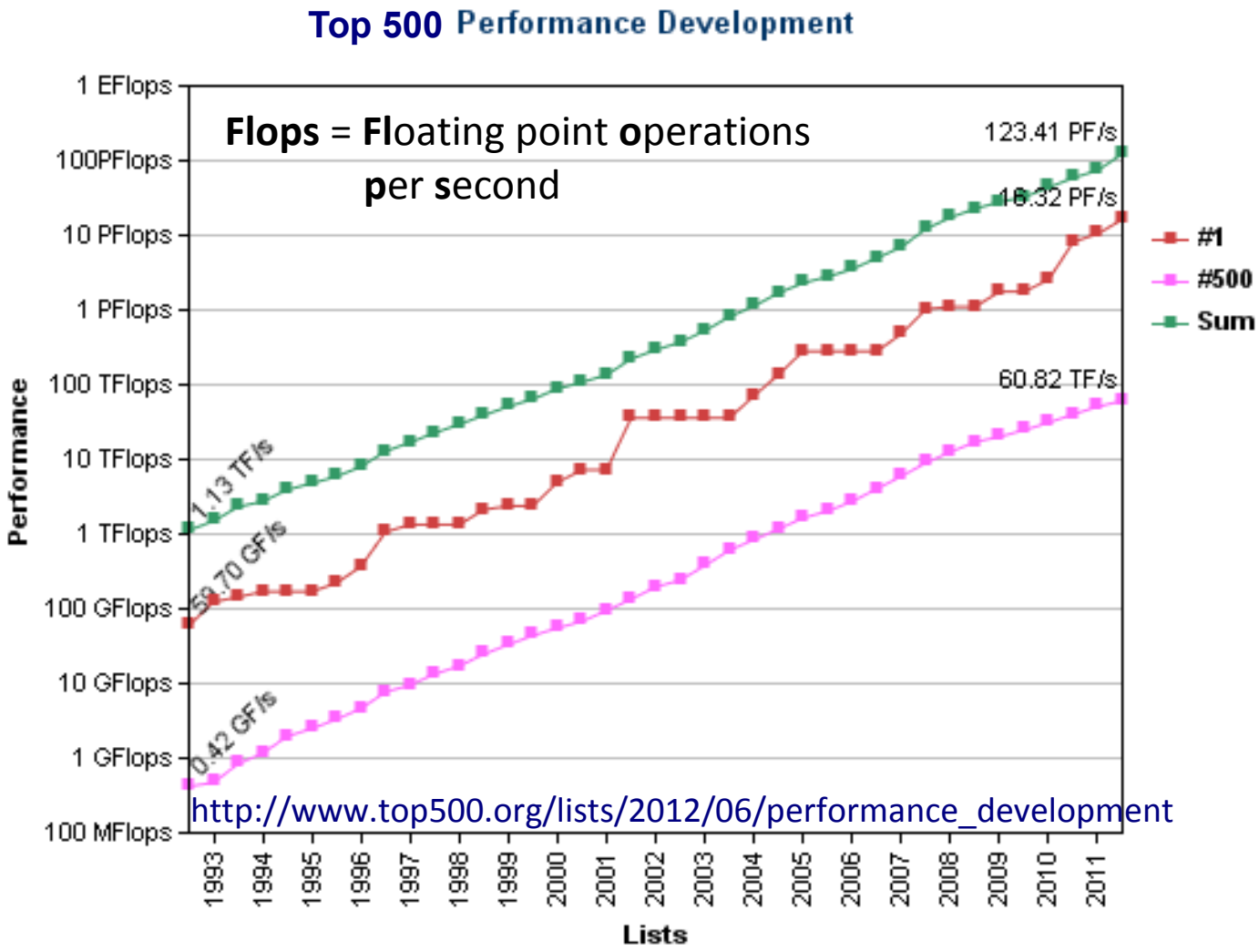
- Motivation for scientific computing
- Creating account at the Usha machine
- Using Usha: “Hello world!” in FORTRAN
- Linux 101
- Elective seminar 

Why care about computational science (CS)?

- **1. Almost all problems you encounter in real life mandate a numerical approach.** Analytical solution – simplified first estimate, and necessary to understand for designing a proper computational description.
- Computing has grown rapidly in past decades in raw processing power, algorithmic efficiency, and ubiquity in engineering and science.
- Nuclear engineering lags other disciplines in utilizing high performance computing (HPC) resources → the more reason to get involved!
- Recently many efforts started to close the HPC gap in NE, such as:
  - Consortium for Advanced Simulation of Light Water Reactors (CASL) http://www.casl.org
  - SCALE moves towards HPC, expected in v7. http://scale.ornl.gov/
  - Nuclear Energy Advanced Modeling and Simulation (NEAMS) Program. http://www.ne.doe.gov/AdvModelingSimulation/program.html

Why care about CS? (2)

- Performance growth of top 500 supercomputers remains exponential (Moore's law).
- Today's desktops CPUs ~ 100 GFlops, #500 supercomputer from year 2001.
- Today's desktops GPUs ~ 4.3 TFlops. A modern PC with 2x AMD Radeon HD7970, #1 supercomputer from year 2001.



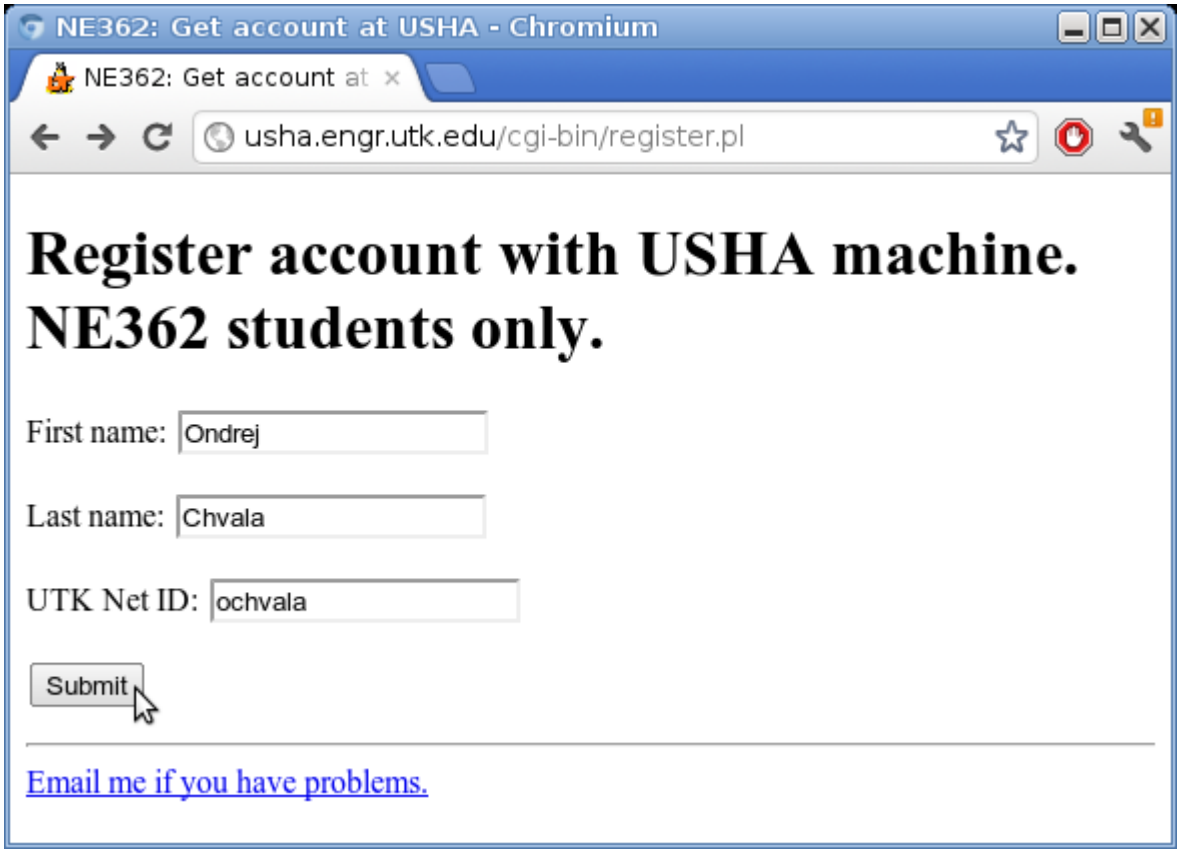
- NB: Raymond Kurzweil estimates human brain power ~ 20 PFlops. BlueBrain project est. 100 EFlops to emulate brain at molecular level.

Why care about CS? (3)

- **2. Analytical thinking and its application to describing and solving problems computationally may likely be your most marketable skill.**
- It will allow you to solve problems in automated fashion, that is more quickly and more efficiently.
- This will be useful not just in a NE career, but in any other field. You never know where life will take you, and computing is everywhere: from basic to applied research, finances, etc.
- Understanding computing allows understanding of cybersecurity, which is becoming more and more issue for private citizens, industry, and government agencies.
- **3. Computing is fun, and useful outside of your professional career:**
  - Home automation, Digital gardening, DIY projects, Self-reliance, …

Creating account at Usha box

- **During the course, you will learn to program in FORTRAN. Usha is a play machine for you.**
- Not fast but sufficient :-) P4/3.4GHz, 1GB RAM, Debian Linux
- To create an account: http://usha.engr.utk.edu/cgi-bin/register.pl
- Fill in your name and netid, click “Submit”, and you will get email with a link to click, see next slide.



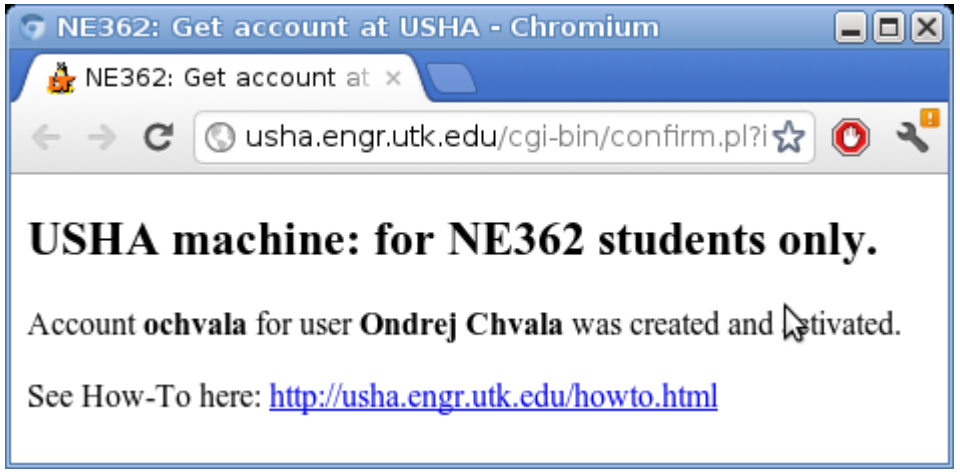
Creating account at Usha box (2)

- You will get an email, click on the link:

From o@usha.engr.utk.edu
Subject **Create account at usha.engr.utk.edu**
To Me <ochvala@utk.edu>

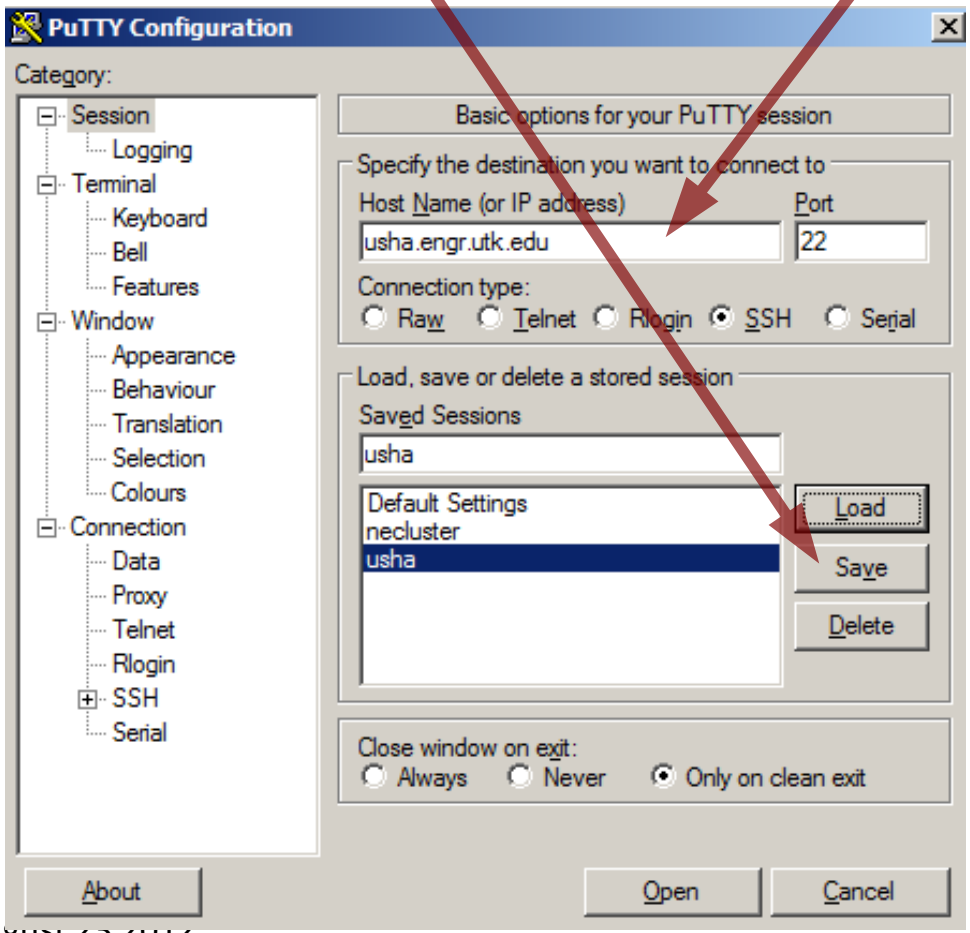
```
Hi Ondrej Chvala!

Your account at usha.engr.utk.edu will be activated by clicking at this link:

http://usha.engr.utk.edu/cgi-bin/confirm.pl?i=d8942f85a609aae2510493dc33087e45

You can also copy the above link to a browser.


Your login name is: ochvala and your password is: dLbA7fCj
Please change your password.

For a simple how-to get started on the Usha system see here:
http://usha.engr.utk.edu/howto.html

Regards,
Ondrej Chvala
```

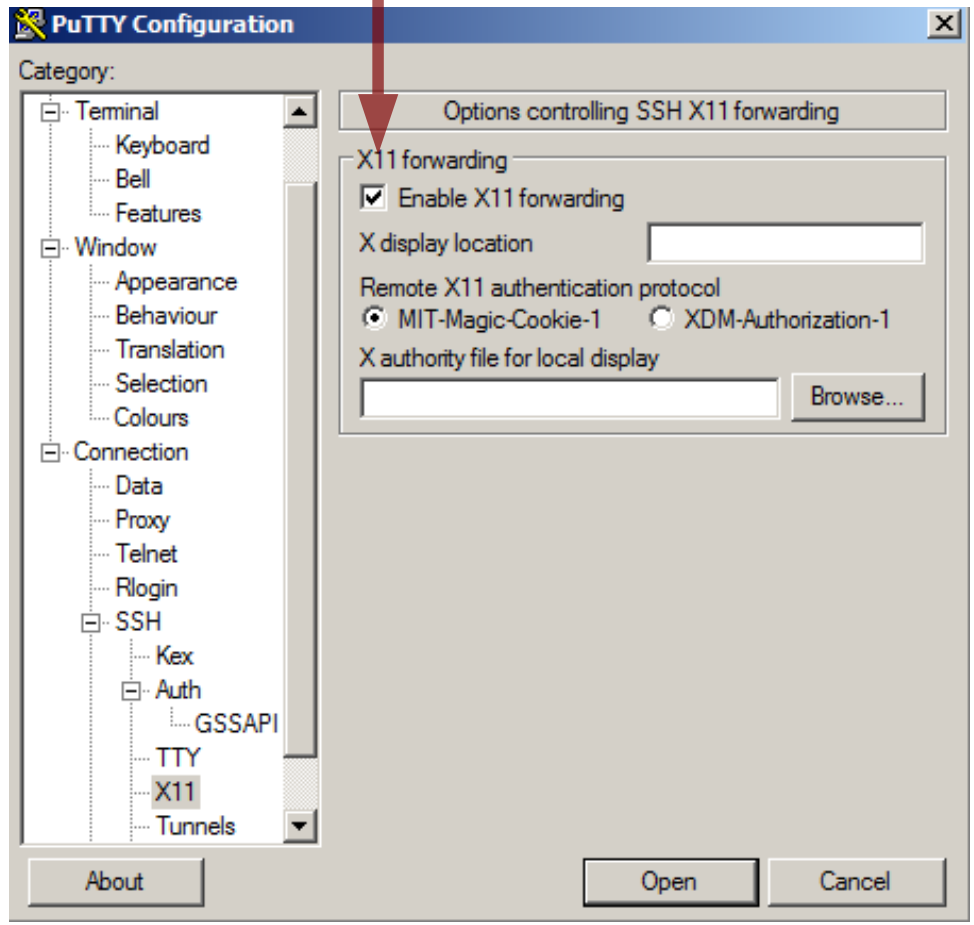
- After you click, the account is activated:



Connecting to Usha

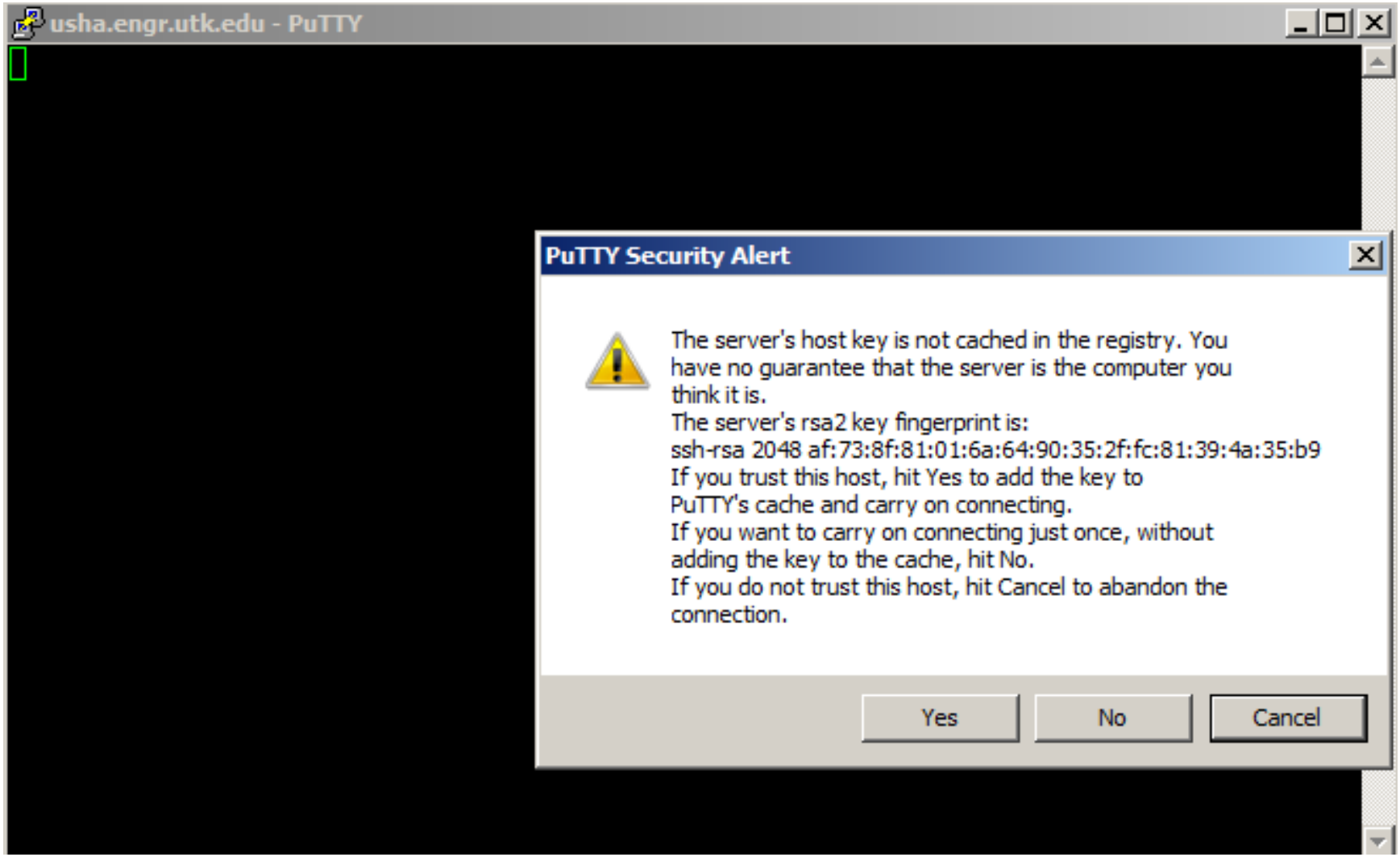
- You need an ssh client. For Linux and MAC use ssh command, for Windows download PuTTY: (Google PuTTY) http://www.chiark.greenend.org.uk/~sgtatham/putty/download.html
- Put “usha.engr.utk.edu” into Host Name, enable X11 forwarding, save session





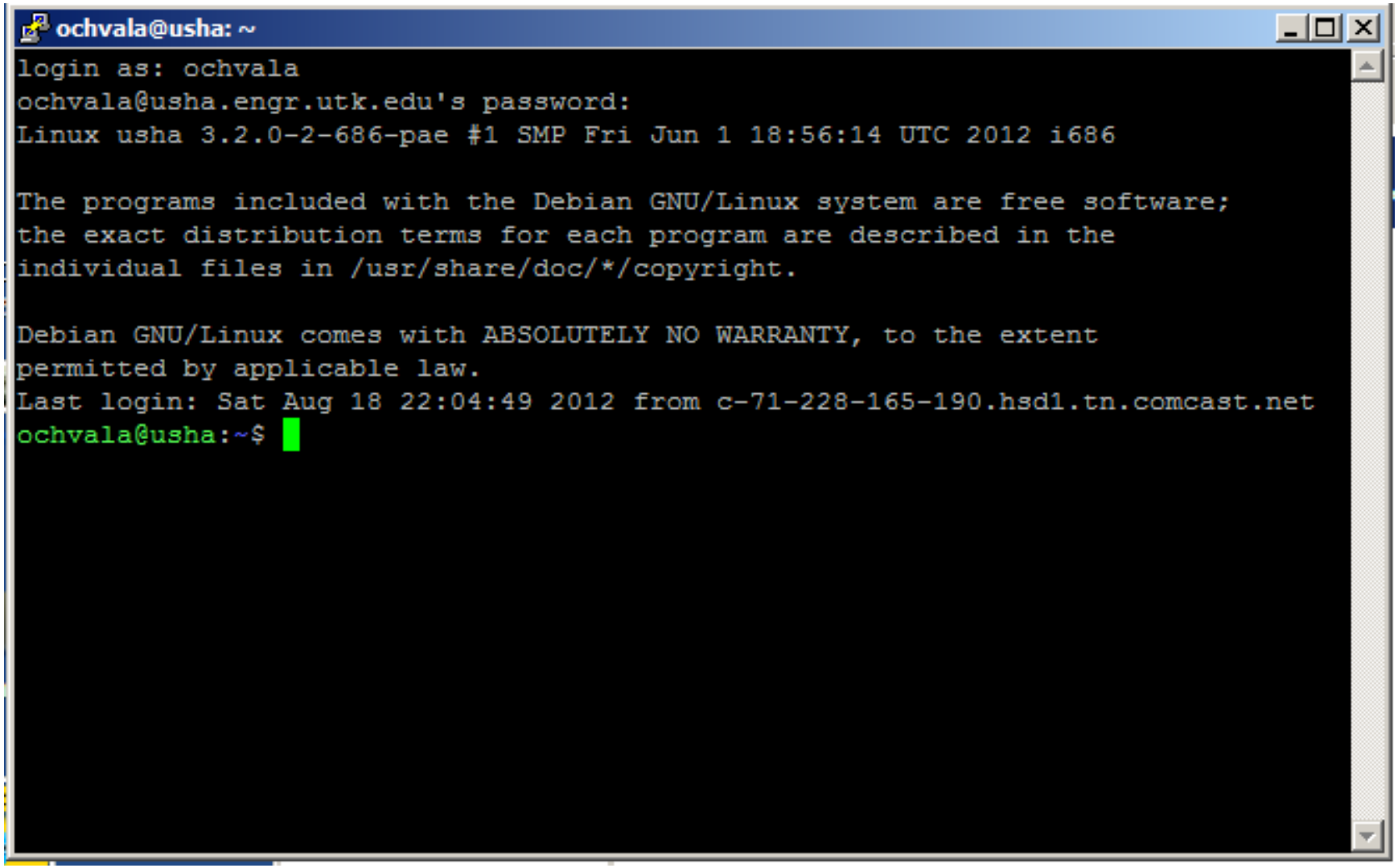
Connecting to Usha (2)

- Click Connect, confirm ssh server key:



Connecting to Usha (3)

- Type your username and password, and you are in:



- **Change your password using *passwd* command!**

Compiling test program “HelloWorld”

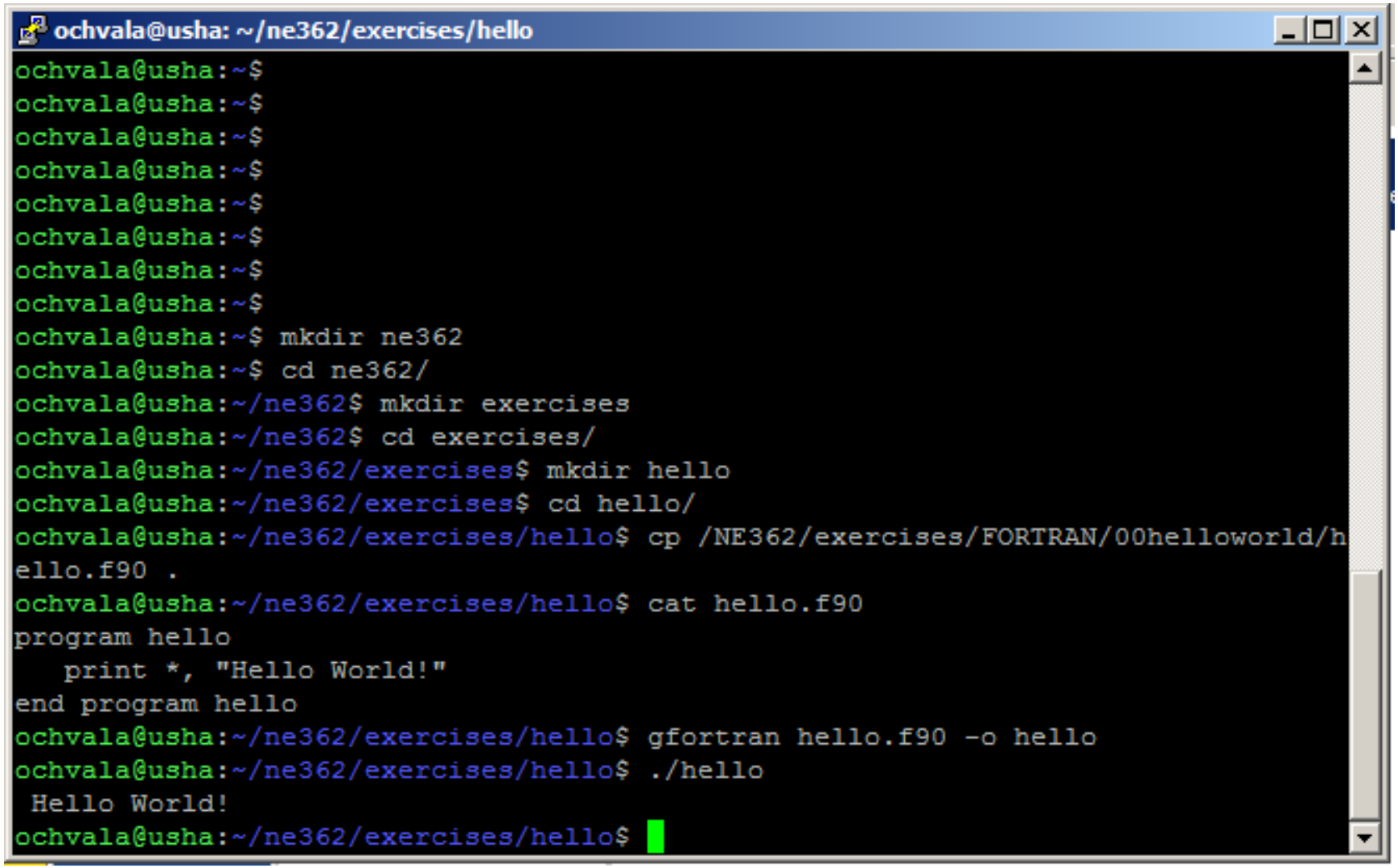
- First lets create a play directory, and cd there:
  - *mkdir -p ne362/exercises/hello*
  - *cd ne362/exercises/hello*
- Now lets copy the program over: (the last dot “.” means current dir)
  - *cp /NE362/exercises/FORTRAN/00helloworld/hello.f90 .*
  - *cat hello.f90*
- Compile the code using *gfortran* and run it:
  - *gfortran hello.f90 -o hello*
  - *./hello*
- You should see: **“Hello World!”**

hello.f90:

```
program hello
   print *, "Hello World!"
end program hello
```

Compiling test program “HelloWorld” (2)

- Here is the above in terminal:



Navigating around a Linux box

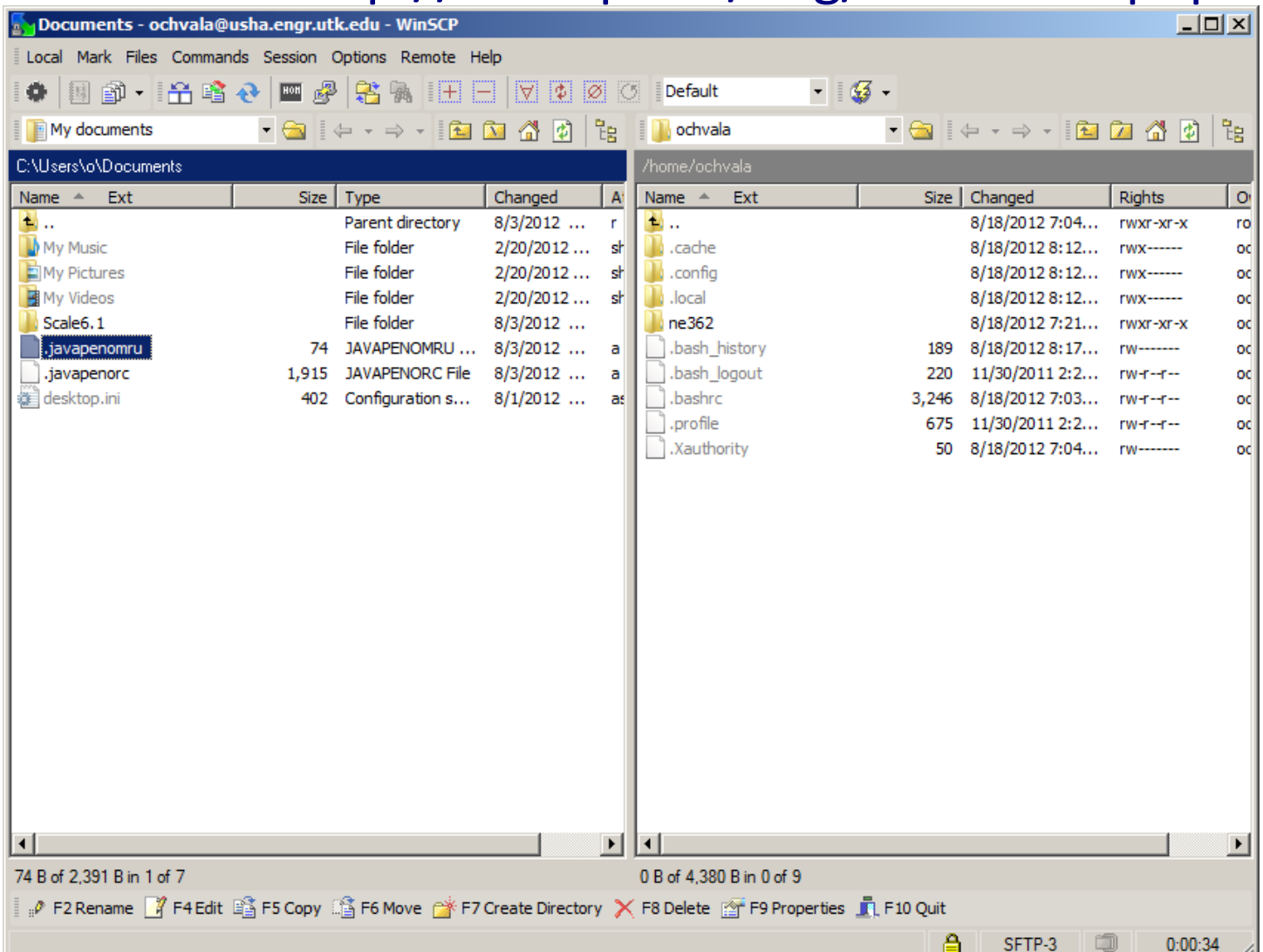
- List files in a directory: *ls -lah*
- Copy file: *cp <from> <to>*
- Move file: *mv <from> <to>*
- Remove file: *rm <file>*
- Need help? Use *man <command>,* Google is your friend.
- See “resources” links at http://usha.engr.utk.edu/welcome.html
- Midnight Commander (command *mc*) is a useful tool to navigate around a Linux computer, similar to Norton/Far/Volkov Commanders.
  - View/change directory, view/edit/copy/move files, ...

Copying files to/from Usha

- From Linux/Mac use scp command: *scp <from> <to>*, such as:
  - *scp thisfile ochvala@usha.engr.utk.edu:*

man scp

- Windows: use WinSCP http://winscp.net/eng/download.php



Other ways to get Linux

- You can run Linux on your own machine in several ways:

  a) boot from LiveCD or LiveUSB drive – slower, least work

  b) install it as the only OS – say if you have an old unused computer

  c) shrink Windows partition and install it as a dual-boot option

  d) install Linux into a virtual machine:

    - download VirtualBox from https://www.virtualbox.org/ (supports Windows, Linux, Mac, Solaris host OS)
    - configure virtual machine, install Linux on it.

- Which Linux flavor to choose? I would suggest Ubuntu or its derivatives, just for the sake of popularity: easy to get help on-line.
- Ubuntu: http://www.ubuntu.com/download
- Linux Mint: http://www.linuxmint.com/download.php

Summary thus far

- Computing is important for your career, in particular in research, in particular in NE now. Importance will increase in future with growing computational ability.
- High performance computing (HPC) uses Linux – learn it, love it.
- We have a play Linux machine for you (usha.engr.utk.edu). Use it.
- Familiarize yourself with basic command line. Helpful command *man*.
- There are plenty Linux resources on-line. Google.
- Get your own Linux: USB stick, virtual machine, separate computer, dual-boot.

Elective seminar

- Due to popular demand, there will be a voluntary seminar covering practical aspects of CS. This would be useful to you in a graduate school, NE related research, or carriers outside of NE.
- Seminar topics: introduction to high performance computing, basic Linux, useful practical tools such as bash or perl scripting, basic C/C++, using an object oriented framework such as ROOT. This is a suggestion and I welcome your input. If you have a particular interest in other topic(s) I am familiar with, I would be willing to make a lecture covering it. Email me suggestions.
- Everything would be covered on a "get me started" level, such that you could independently explore a topic of your interested in depth.
- We could also do exercises related to NE362 syllabus.
- **Seminar time: Thursdays, 5:05pm – 6:35pm, Pasqua bldg. room 206**