# HPC Account and Software Setup

# Ken-ichi Nomura

### MAGICS 2<sup>nd</sup> Workshop at USC March 2, 2018





# **1. USC Secure Wireless** 2. eduroam 3. MAGICS@USC password: magics@usc 4. USC Guest Wireless

# **Software Setup**

- To access the USC HPC cluster, we need virtual terminal, ssh & scp client for remote login and transfer files.
- This slide will show you how to install Putty & FileZilla for Windows and Mac users, but you can also use any software you are familiar with.





Putty http://www.putty.org FileZilla https://filezilla-project.org

# **Putty Setup (Windows users only)**

- Go to Putty website <u>http://www.putty.org</u>, then click the download link.
- After a new page opens, choose MSI('Windows Installer') 64-bit link.
- 3. It will download the Putty installer executable. Double click the installer.



#### Download PuTTY

PuTTY is an SSH and telnet client, developed origina that is available with source code and is developed



Package file	25			
You probably (Not sure when	want one of these. They include all the Pul	TTY utilities. on? Read the <u>FAQ entry</u> .		
MSI ('Windo	ws Installer')			
32-bit:	putty-0 70 installer msi	(or by FTP)		
64-bit:	putty-64bit-0.70-installer.msi	(or by FTP)		
Unix source archive				
.tar.gz:	putty-0.70.tar.gz	(or by FTP)		

# **Putty Setup (Windows users only)**

🕵 PuTTY Configuration	? 🗙
Category:	
Session     Logging     Terminal     Keyboard     Bell     Features     Window     Appearance	Basic options for your PuTTY session Specify the destination, a swant to connect to Host Name (or IP address) Port 22 Optimection type. Raw Contract Rilogin © SSH © Serial Load assesses
Behaviour Translation Selection Colours	Load, save or delete a stored session Saved Sessions
⊡ ·· Connection ···· Data ··· Proxy ··· Telnet ··· Rlogin ⊕·· SSH	Load Save Delete
About Help	Close window on exit: Always Never Only on clean exit Open Cancel

### Host Name: hpc-login3.usc.edu

In "Hostname (or IP address)" box, type hpc-login3.usc.edu , then click "Open" button.

# **Putty Setup (Windows users only)**

• You will be asked to type your username, e.g. **magics35**, and password.



• Each of us uses one account through this workshop, so please do not lose your login information, or share with your friends.

# How to Use Terminal (Mac users only)

- For Mac users, a virtual terminal called **Terminal** is available by default. No need to install anything.
- Either search it with **Spotlight** or go to /**Applications/Utilities** directory.



# How to Use Terminal (Mac users only)



- Open Terminal, then type ssh username@hostname from command line. For example, \$ssh magics35@hpc-login3.usc.edu
- You will be asked to type password. Type in your password, then press **Enter** key. That's it!

# FileZilla Setup (Windows and Mac users)

- There are four boxes you need to type in. 1-Hostname, 2-Username, 3-Password, and 4-Port.
- Port is always **22**.

🔁 FileZilla							- • -
File Edit View Tr	ransfer Server	Bookmarks He	elp				
📃 🕶 🚺 🗉 😷	🗲 🗱	P3 💺 🛷 🗐 📰	R 6	ñ			
Host fipc-login3.us	sc.edt Isernam	ne: knomura	Pas	sword:	••• P	ort 22	Quickconnect 💌
							*
							-
Local site: C:\Users\kn	omura\Desktop\		-	Remote site:			
Filename	Filesize	Filetype	Last m	Filename	Filesize	Filetype	Last modified
J							
🛍 desktop.ini	282	Configuration	8/30/2				
🔁 FileZilla.Ink	1,044	Shortcut	8/30/2		Not connect	ted to any serve	r
PuTTY.Ink	857	Shortcut	8/30/2				

Host: hpc-login3.usc.edu Username: magicsXX

# FileZilla Setup (Windows and Mac users)

Unknov	vn host key
1	The server's host key is unknown. You have no guarantee that the server is the computer you think it is.
	Host: hpc-login2.usc.edu:22 Fingerprint: ssh-rsa 1024 f6:82:b8:44:a0:58:fe:ae:89:fb:8a:10:86:be:5a:ca
	Trust this host and carry on connecting?
	OK Cancel

- When you access a remote server first time, you will be asked to accept its host key, or not.
- Click **OK**.

# FileZilla Setup (Windows and Mac users)

- Once you successfully log on the remote computer, you will see local files (red) and remote files (blue).
- You can drag&drop to transfer files between local and remote computers.

N 🕈 💭 🗉 😭 😴 🗱 🕺 🏁 🗽 🛷 💷 📯 🦻 🛝							
Host: sftp://hpc-log	Host: sftp://hpc-login2.usc. Username: knomura Password: •••••• Port: Quickconnect						
Response: 1363198720 Status: Timezone offsets: Server: -25200 seconds. Local: -25200 seconds. Difference: 0 seconds. Status: Directory listing successful					*		
Local site: C:\Users\knomura\Desktop\   Remote site: /auto/rcf-12/knomura							
Filename	Filesize Filety	pe Last m	c Filename	Filesize	Filetype	Last modified	<u>-</u>
J			<b>.</b>				μ
🗑 desktop.ini	282 Confi	guration 8/30/2	0 📗 .config		File folder	8/9/2013 3:20:0.	
E FileZilla.Ink	104 Short	cut 8/30/2	0 📗 .dbus	Kel		6/26/2013 5:21:.	
PuTTY.Ink	857 Short	cut 8/30/2	0 📗 .eclipse		File folder	4/11/2013 2:53:.	
	Computer						
	mpate		퉲 .felix		F. le folder	8/22/2013 5:39:.	
			퉲 .fltk		File folder	2/9/2006	
			퉲 .fontcon.		File folder	9/1/2013 2:46:0.	
			📗 .gconf		File folder	8/20/2013 3:01:.	
			📗 .gconfd		File folder	8/20/2013 3:06:.	Ŧ

## **Visualization & Analysis Software**

#### **VMD: Visual Molecular Dynamics**

http://www.ks.uiuc.edu/Research/vmd/



VMD is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting. VMD supports computers running MacOS X, Unix, or Windows, is distributed free of charge, and includes source code.

(more details...)

#### Spotlight

Recent improvements to the data structures and algorithms used to display and analyze molecular structures in VMD have improved it's utility in **bionanotechnology**, and materials science where large structures, various types of non-biological matter, and non-polymeric structural elements are often present.

#### **Other Spotlights**



## **VMD Setup**

# Click **Download VMD** link on the left, then choose platform for your OS in **VMD Version 1.9.3 (2016-11-30) Platforms**.

Graphics viewer		
NAMD Molecular Dynamics Simulator	Spotlight	
<ul> <li>BioCoRE Collaboratory Environment</li> </ul>	Dr. Oliver Beckstein's VMD image was voted the picotinic acetylcholine recentor. The imag	Version 1.9.3 (2016-11-30) Platforms:
MD Service Suite	1.8.3 and rendered with Raster3D 2.7c.	
<ul> <li>Structural Biology Software Database</li> </ul>	Other Spotlights	We recommend that all users upgrade to VMD 1.9.3
Computational Facility		
Outreach	Quantan	Source Code
	Overview	INUX 64 OpenGL_CUDA_OptiX_OSPRay (Linux (RHFL)
	Molecular representations	LINUX_C4 Text mode w/ FOL (Linux (DUEL C 7 and later)
VMD	VMD plugin library	• LINUX_64 Text-mode w/ EGL (LINUX (RHEL 6.7 and later)
Mailing	GPU-accelerated computing	<ul> <li>LINUX 64 Text-mode (Linux (RHEL 6.7 and later) 64-bit In</li> </ul>
	Interactive molecular dynamics	• I INUX MIC-AVX512 Text-mode (Linux (RHFL 67 and late
Download	Programs that use VMD VMD research publications	
VIIID	How to cite VMD	• LINUX MIC-AVX512, OpenGL, CUDA, OptiX, OSPRay (LI
VMD	VMD citation list (19,000 as of Oct'16)	<ul> <li>LINUX OpenPOWER Text-mode (Linux 64-bit IBM OpenP</li> </ul>
Tutorials	Download	MacOS X OpenGL (32-bit Intel x86) (Apple MacOS-X (10)
VMD		
Manuals	Download (all versions)	Windows OpenGL, CUDA (Windows XP/Vista///8/10 (32-b)
VMD	VMD 1.9.3 (MacOS X, Unix, Windows)	<ul> <li>Windows OpenGL (Microsoft Windows XP/Vista/7/8/10 (32)</li> </ul>
Community	VMD 1.9.1 (MacOS X, Unix, Windows)	NCSA Blue Waters (Cray XK7 w/ OpenGL) (NCSA Blue V
Pages	VMD script library	INCOA Blue Waters (Cray XK/ W/ OpenGL) (INCOA Blue V

Your platform is most likely LINUX\_64 OpenGL, MacOS X OpenGL (32-bit Intel x86), or Windows OpenGL.

# **VMD Setup**

- Simple registration is required to download VMD.
- Type username and password, then click **Continue with** registration or download.

Registration/Login	
You will need a username and password	to download software.
f this is your first download, please ch Current NAMD or VMD users, please ente	oose a username and password to register. er your existing username and password.
Jsername:	
Password:	
Continue with registration or download	

• You will be asked a few more questions. Click the VMD license agreement button, then you will download a VMD installer with the executable.

## **Visualization & Analysis Software**

### OVITO: Open Visualization Tool https://ovito.org



# **OVITO Setup**

• Click **Download** tab on top. Choose your OS, then click download link.

Home       About       Download       Documentation       Forum       Contact         OVITO is available free of charge under the terms of the GNU General Public License. Please cite OVITO when you publish any results obtained with it.         Program packages			
Operating system	Current stable version (27-Jul-17) Development version (30-Oct-17) Info		
👃 Linux	Download OVITO 2.9.0	OVITO 3.0.0-dev53	
Windows	Download OVITO 2.9.0 (installer   zip archive)	OVITO 3.0.0-dev52 (installer   zip archive)	
macOS	Download OVITO 2.9.0	OVITO 3.0.0-dev52	

# **USC HPC Environment Setup**

- USC HPC cluster has setup scripts (**setup.sh**) under /**usr/usc** directory to enable installed software and libraries.
- We are going to use Intel Fortran Compiler and OpenMPI library, Python Anaconda in the hands-on sessions.
- Copy dot.bashrc file to your home directory as .bashrc.

#### \$ cp ~magics35/magics/dot.bashrc ~/.bashrc

• Make sure you have following lines in your .bashrc file.

```
$ cat ~/.bashrc
#
...
source /usr/usc/intel/default/setup.sh
source /usr/usc/openmpi/default/setup.sh.intel
source /usr/usc/python/anaconda3/setup.sh
```

# Acknowledgement

This work was supported as part of the Computational Materials Sciences Program funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Award Number *DE-SC00014607* 

Materials software (Thermal Conductivity Plugins for LAMMPS, RXMD, QXMD, GEARS) used in this research was produced by USC MAGICS Center that is a part of the Computational Materials Sciences Program funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Award Number *DE-SC00014607*.



