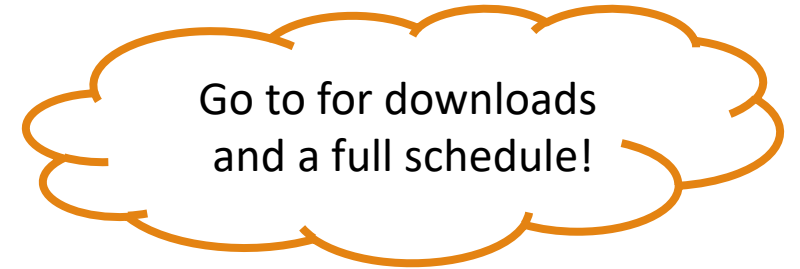


# HPC Workshop 2022

*Upward Bound*



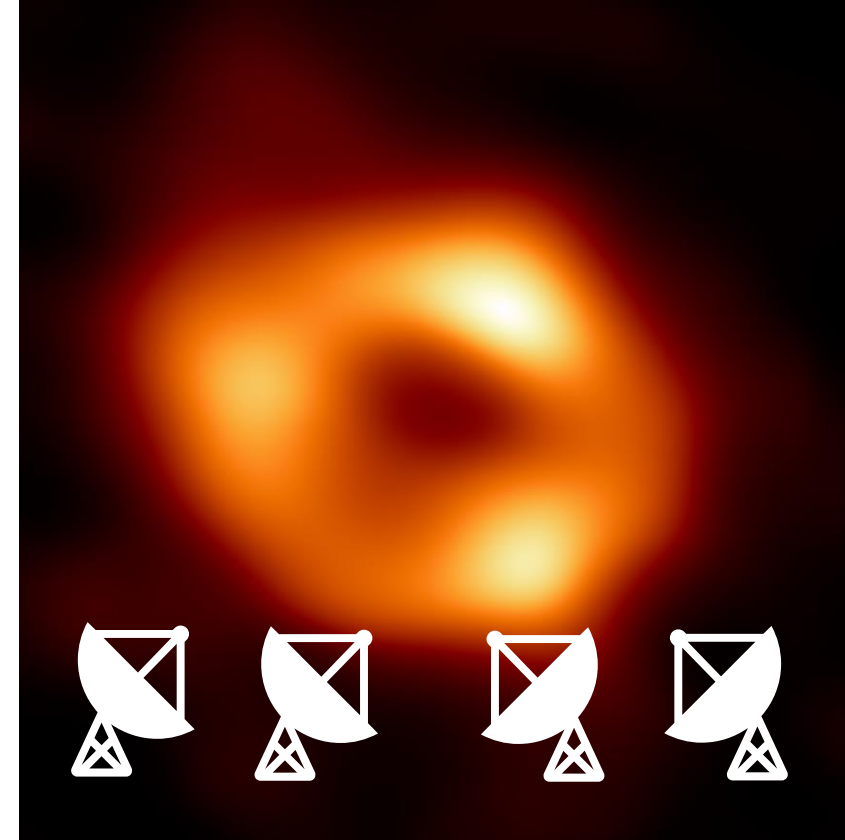
<https://uwec.ly/hpcworkshop>



**Please log into your machine when you take a seat.**

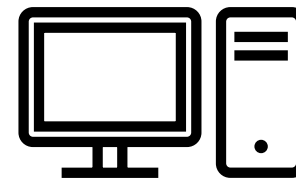


Imagen:  
A small cactus wearing a straw hat and neon sunglasses in the Sahara desert.



What do these have in common?

Computers!



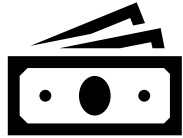
# Computational Science

---

*USING COMPUTERS... FOR SCIENCE!*

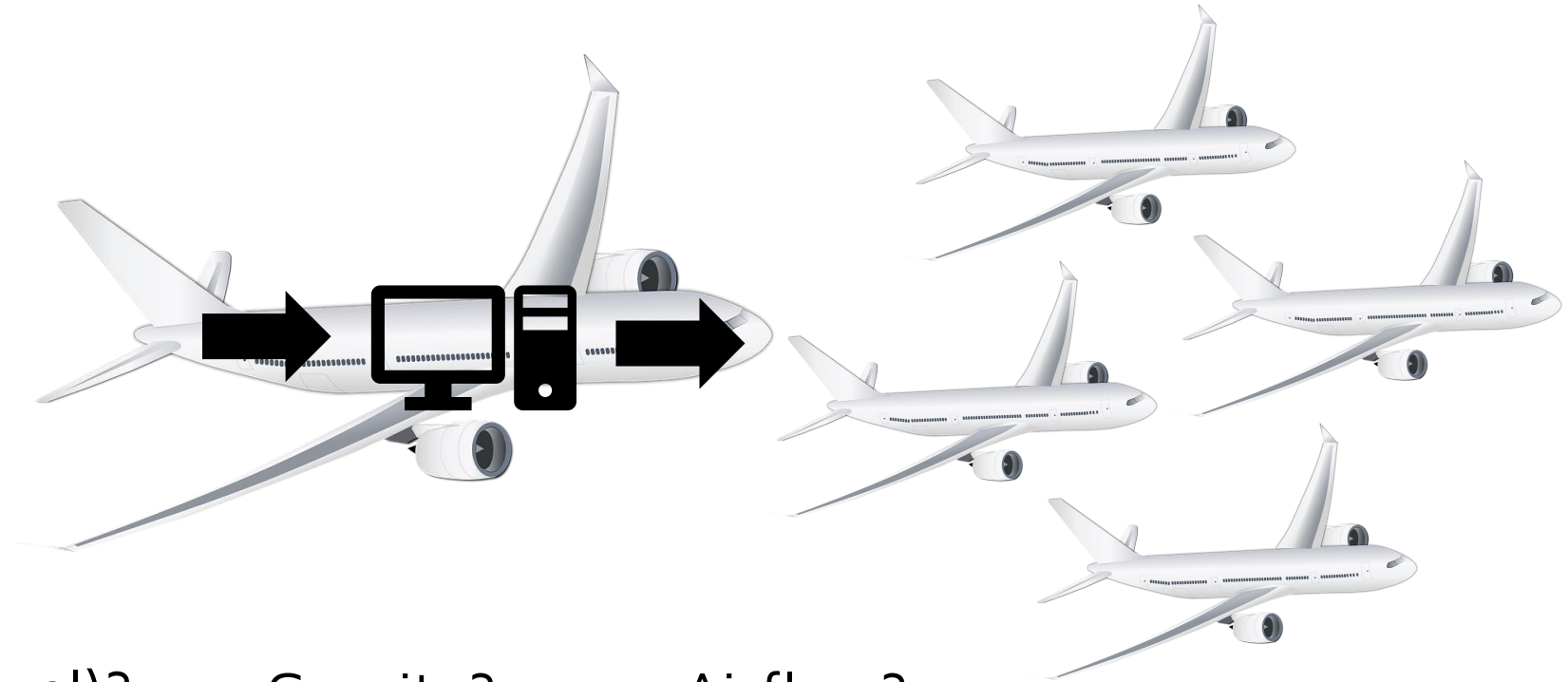
# Imagine

---



# Computational Science

---



Weight (+Fuel)?

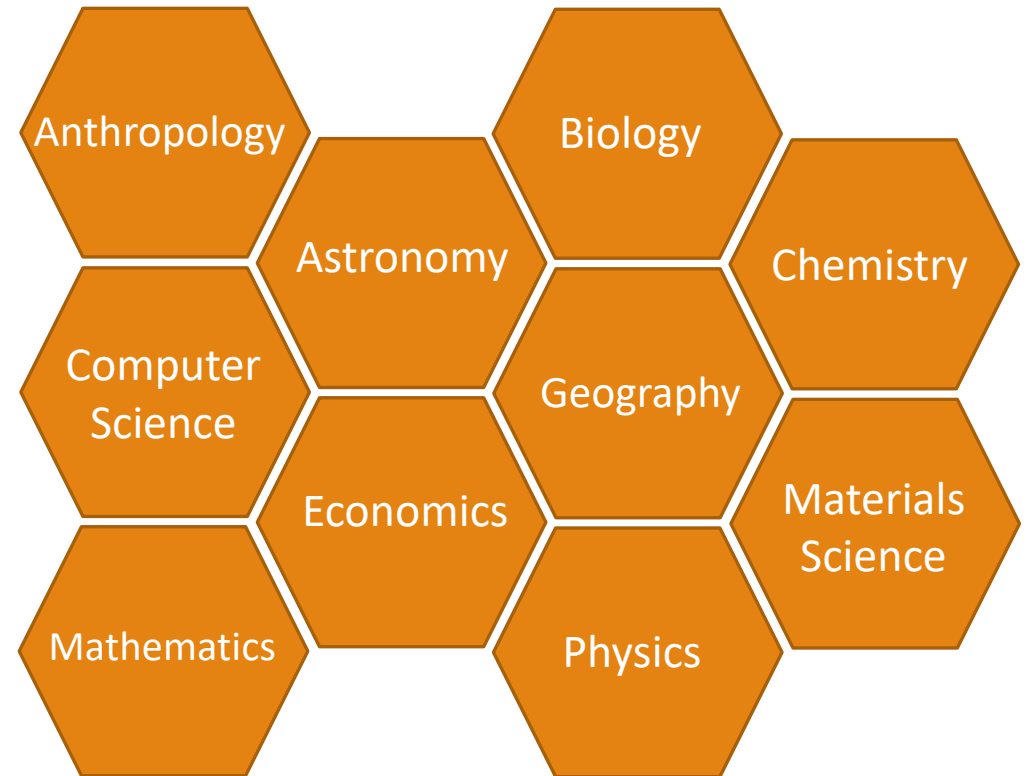
Gravity?

Airflow?

# Computational Science

---

- Complex Math
- Simulations
- Analysis
- Computers



And so much more...

# Computational Science

---

- *Autonomous cargo ship completes first ever transoceanic voyage – 6/06/2022 – The Independent*
- *Great timing, supercomputer upgrade lead to successful forecast of volcanic eruption – 6/3/2022 – UIUC*
- *Astronomers Reveal First Image of the Black Hole at the Heart of Our Galaxy – 5/12/2022 – NRAO*
- *Using AI, Stanford Researchers Develop An Algorithm To Detect Illegal Deforestation With The Help Of Satellite Images – 4/27/2022 – MarkTechPost.com*

# High Performance Computing (HPC)

---

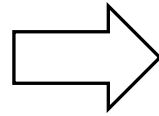
MORE POWER!



*"I need to do multiple sampling events of multiple simulations. No way can my existing system pull that off in a timely fashion, if at all."*

*~David Warner, Research Fisheries,  
Biologist*

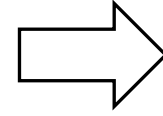
Personal



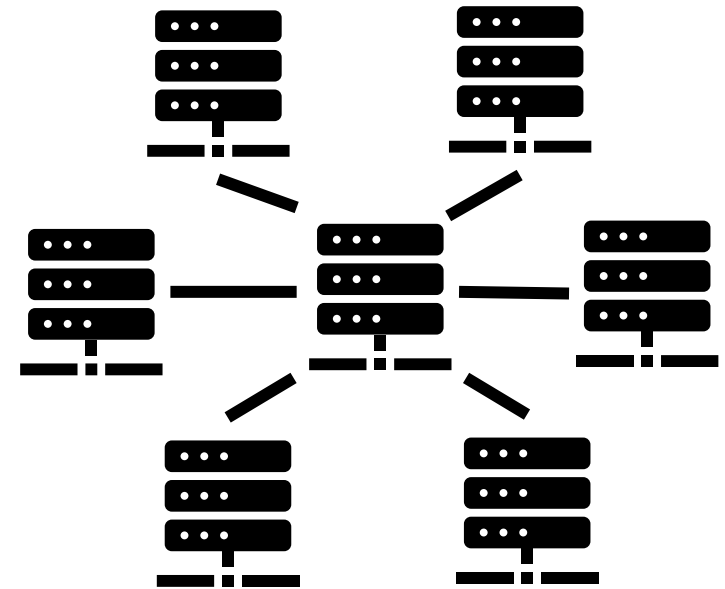
Supercomputer



One



Supercomputing  
Cluster



Many

High-Performance Computing

# Fugaku in Japan

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© Riken Research Institute

158,976 Nodes (Machines)! - \$1 Billion

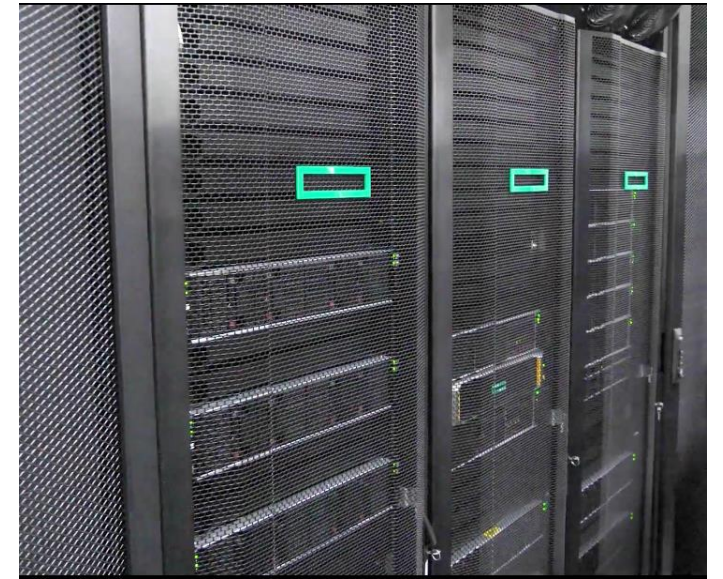
# Blugold Center for HPC

---

# HPC @ UWEC

---

- UWEC has two clusters (BGSC and BOSE)
  - Approx 85 machines combined
- Only one of three schools in the UW System
  - Madison
  - Milwaukee
  - Eau Claire
- Available to all faculty, staff, and students



BOSE

## BGSC



Primarily used for classrooms  
20 Machines

*You're going to use this!*

## BOSE



Primarily used for research  
60 Machines

# The Team

---

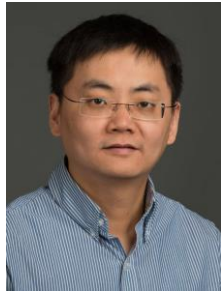
## Faculty Coordinators



Dr. Sudeep  
Bhattacharyay



Dr. Rahul  
Gomes



Dr. Ying  
Ma

## System Administrator



Tyler  
Bauer

## Management



Kent  
Gerberich



Tom  
Sulzer

## Student Administrator Apprentices



Mitchell  
Ewan



Treesmorn Tanboonrith  
"Mammoth"



Jacob  
Weber

# Who uses us?

---

- Classroom use
- Research Projects
- Departments
  - Biology
  - Chemistry & Biochemistry
  - Computer Science
  - Geography
  - Materials Science & Biomedical Engineering
  - Physics
  - *And More*

University of Wisconsin  
**Eau Claire**



# The Workshop

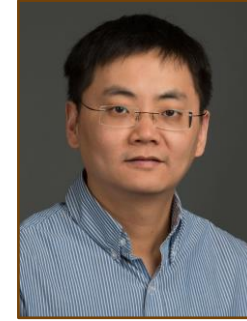
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Sudeep Bhattacharyay, Ph.D.  
Chemistry / Biochemistry  
Associate Professor



Rakib Islam, Ph.D.  
Computer Science  
Assistant Professor



Ying Ma, Ph.D.  
Materials Science and  
Biomedical Engineering  
Associate Professor



Nora Mitchell, Ph.D.  
Biology  
Assistant Professor



Wufeng Tian, Ph.D.  
Mathematics  
Associate Professor



Bill Wolf, Ph.D.  
Physics + Astronomy  
Assistant Professor

# Today

---

Time	Who	What
9:00 – 10:15	Blugold Center for HPC	Introduction to high performance computing (HPC), computational science, and basic Linux commands
10:30 – 12:00	Dr. Sudeep Bhattacharyay	Making the atoms dance
12:00 – 1:00	LUNCH	LUNCH
1:00 – 2:30	Dr. Nora Mitchell	Building “trees” of South African shrubs – using the HPC to understand evolutionary relationships
2:30 – 2:45	Blugold Center for HPC	Wrap Up

# June 24<sup>th</sup> (Next Friday)

---

Time	Who	What
9:00 – 10:15	Blugold Center for HPC	Recap; Submitting jobs to a supercomputer using Slurm.
10:30 – 12:00	Dr. Bill Wolf	The Lives of Stars
12:00 – 1:00	LUNCH	LUNCH
1:00 – 2:30	Dr. Wufeng Tian	Cryptocurrency Trading Strategies Based on Market Signals and Deep Learning Approach
2:30 – 2:45	Blugold Center for HPC	Wrap Up

# July 8<sup>th</sup>

---

Time	Who	What
9:00 – 10:15	Blugold Center for HPC	Review of high performance computing, Linux commands, and submitting jobs using Slurm.
10:30 – 12:00	Dr. Rakib Islam	How to Teach a Machine to Detect Sentiment - A Machine Learning Approach
12:00 – 1:00	LUNCH	LUNCH
1:00 – 2:30	Dr. Ying Ma	How to engineer a super-bouncy ball
2:30 – 2:45	Blugold Center for HPC	Wrap Up

# Workshop Prep

---

Accessing BGSC2 using:

- WinSCP
- PuTTY

Basic Linux Commands

# Putty | Linux commands | WinSCP

Mammoth

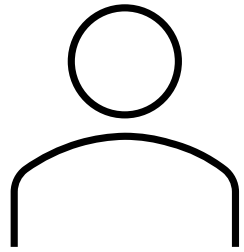
PuTTY

# PuTTY

- SSH (Secure Socket Shell) and telnet client (use application on remote system by server application )
- Open sources software



# PuTTY in nutshell



you

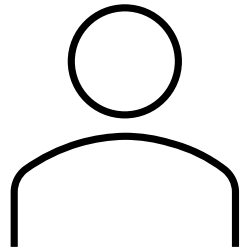


Your login info



BGSC2 Cluster

# PuTTY in nutshell

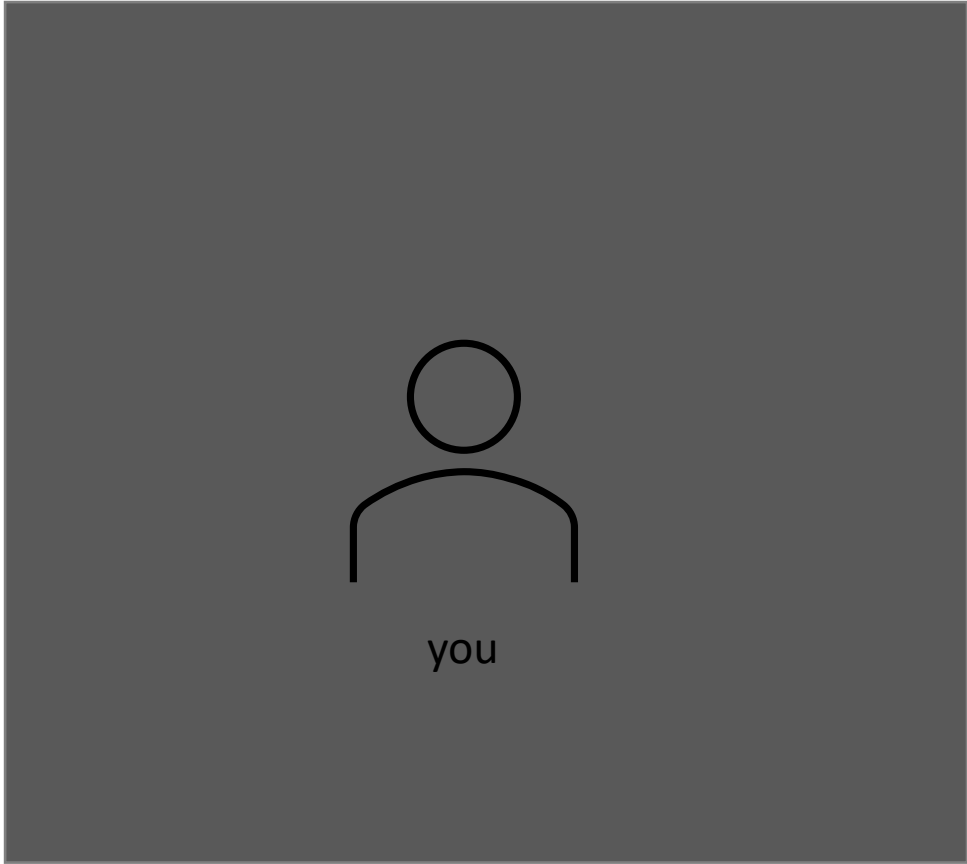


you



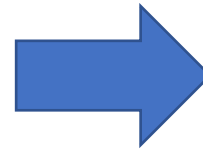
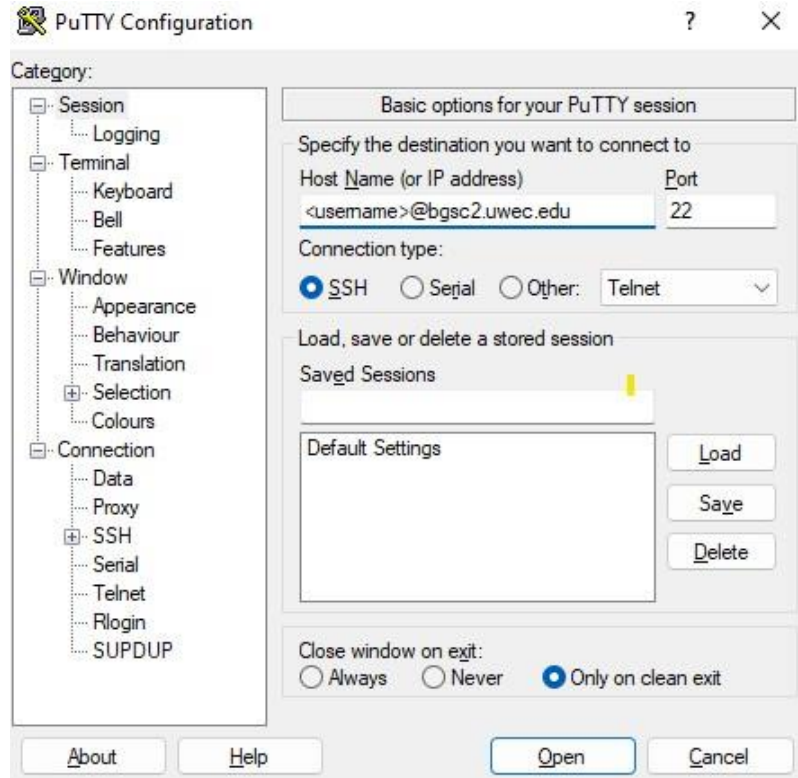
BGSC2 Cluster

# PuTTY in nutshell



BGSC2 Cluster

# PuTTY



Host name: bgsc2.uwec.edu  
Port number: 22  
Username: yourUWECusername

Password: yourUWECpassword

# PuTTY

```
Last login: Thu May 26 16:32:52 2022 from 10.35.27.198

      BGSC2

Policies
-----
1. Any data or files you create on this system are NOT
   backed up.  Users are expected to maintain copies of their
   data elsewhere.

2. Any resource-intensive processes should be submitted
   as Slurm jobs instead of being executed on the head.  Any
   long-standing, resource intensive jobs executed as
   processes on the head node will be terminated.

3. For a list of all our policies please go to https://wiki.bgsc2.uwec.edu/g
   eneral:bgsc-policy
-----

Information and Contacts
-----
For technical or system related questions, please contact:
  BGSC.ADMINS@uwec.edu

BGSC hardware and software information:
  https://wiki.bgsc2.uwec.edu
-----

Node Reservations
-----
The nodes listed below have been reserved for a period of time and are not ac
cessible
while the reservation is active.  They also will not accept any jobs that w
ill not be completed by the Start Date.

Along with the time is what you can use with Slurm's #SBATCH --time=DD-HH:MM:
SS setting to fit jobs in before
```

Successful login to a cluster

# Basic Linux Commands

1. Open Terminal

2. Follow me

# Show the directory and file

1. `ls` (All lower case. No space before and after “ls” )
2. `ls -l` ( All lower case. There is a single space between “ls” and “-l” )

**Note:** The differences between these 2 is that “ `ls -l` ” shows the directory and files in sorted order



# Change the current directory

- `cd` ( All lower case. No space before and after )

# Creating a folder (directory)

- `mkdir` ( All lower case. No space before and after; all lower case )

# Creating a file

- **vi** ( All lower case. No space before and after )
- **vim** ( All lower case. No space before and after )

**Note:** vi is a text editor of Linux. vim is more powerful ( it provides unlimited undo, syntax highlighting, and import configurations for coding a program)

# Show the current working directory

- `pwd` ( All lower case. No space before and after)
- **Note:** “ `pwd` ” stands for print working directory

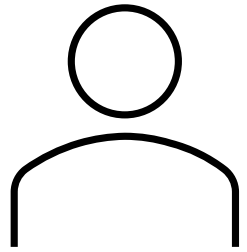
**Note:** Please **DO NOT close PuTTY.** We will use them again

WinSCP

# WinSCP

- SFTP ( SSH files transfer Protocol ) & FTP ( File Transfer Protocol ) for Windows
- Transferring file: You can do drag & drop a file in WinSCP

# WinSCP in nutshell



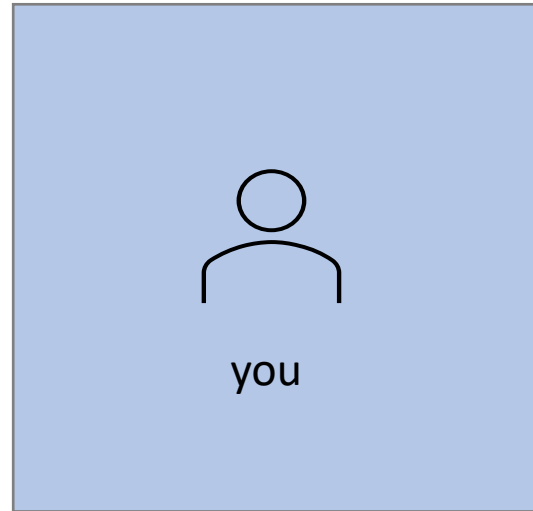
you



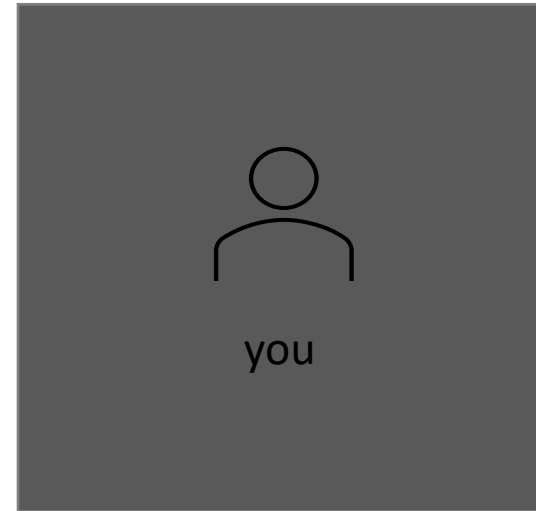
BGSC2 Cluster



# WinSCP in nutshell

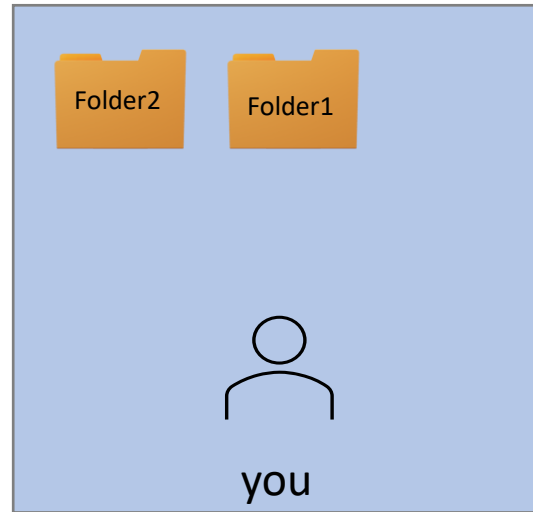


Local machine

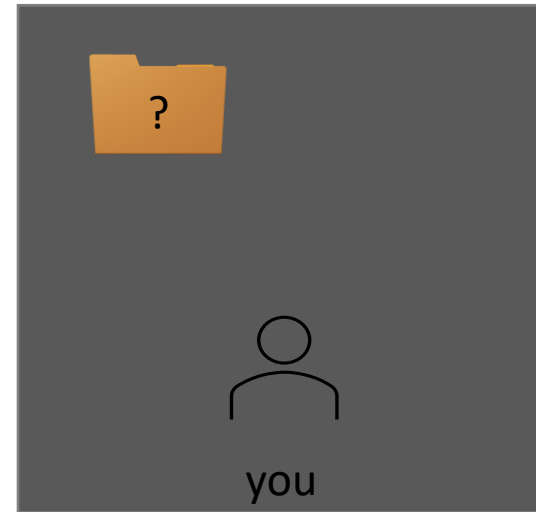


BGSC2 Cluster

# WinSCP in nutshell



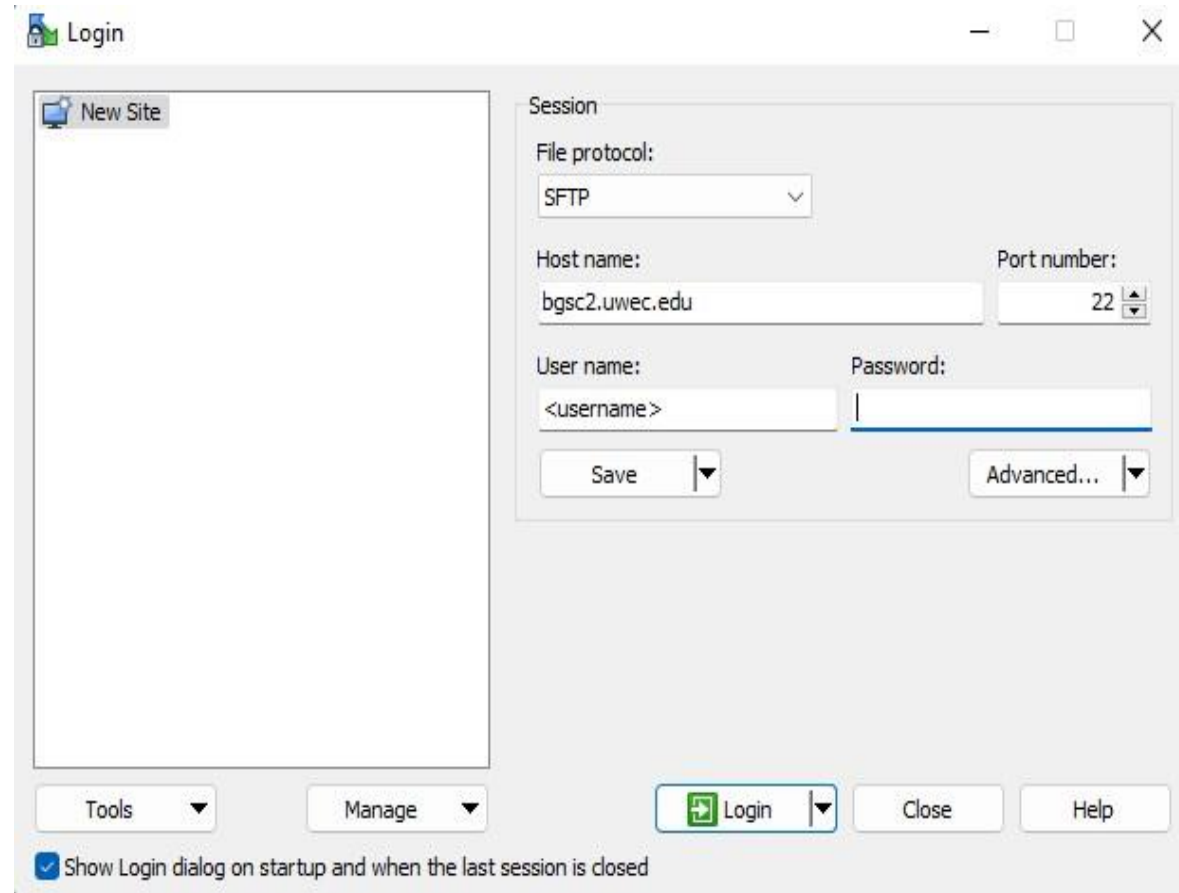
Local machine



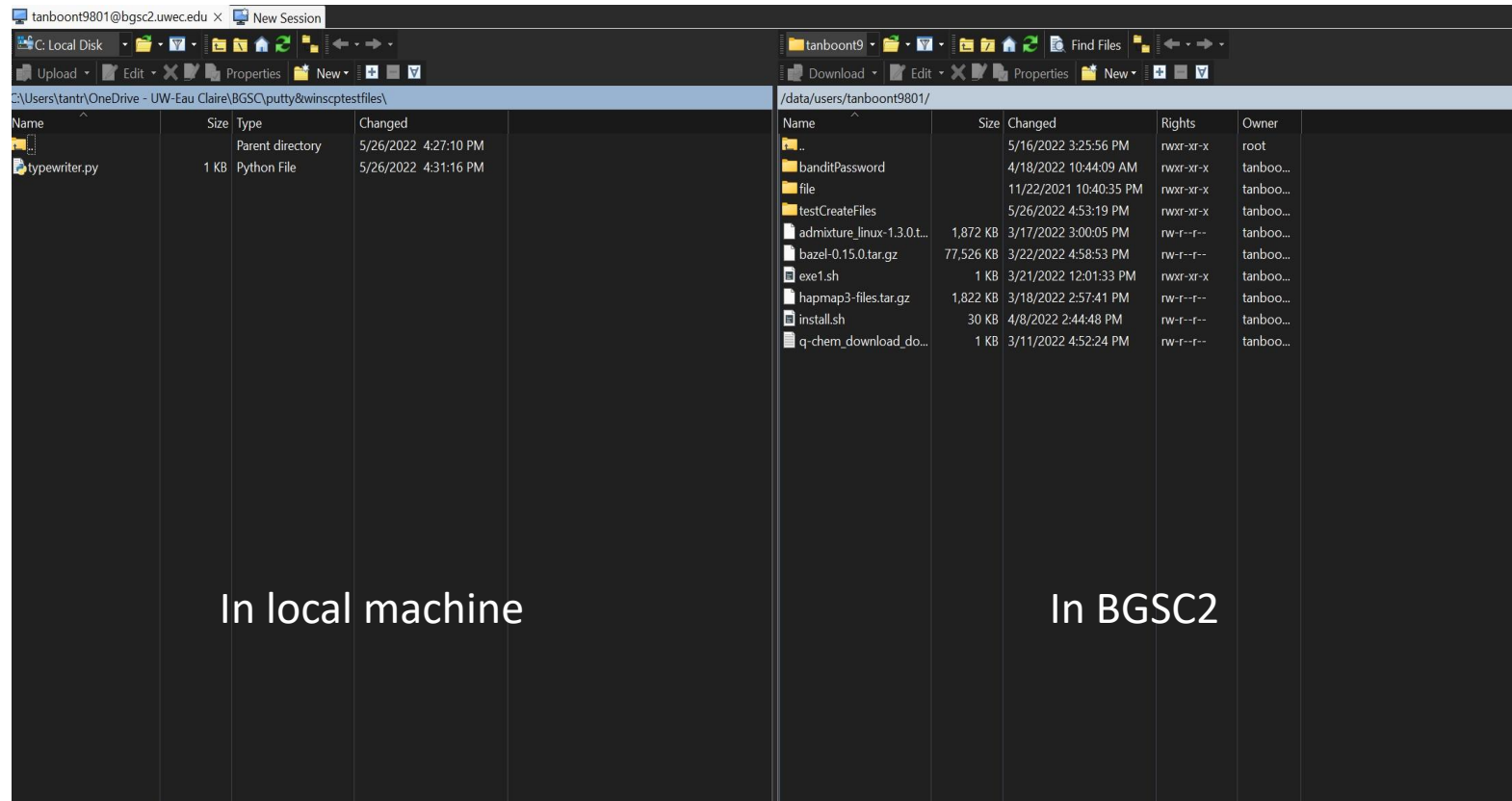
BGSC2 Cluster

# WinSCP

Host name: bgsc2.uwec.edu  
Port number: 22  
Username: yourUWECusername  
Password: yourUWECpassword



# WinSCP



Successful login

# Next Up

---



## Making the atoms dance

---

Dr. Sudeep Bhattacharyay, Ph.D.  
Biology  
Assistant Professor

# Lunch Break

---

BE BACK BY 1:00PM

# Welcome Back! Next Up...

---



Building “trees” of South African shrubs – using the HPC to understand evolutionary relationships

---

Nora Mitchell, Ph.D.  
Biology  
Assistant Professor

**Please log back into your machine.**

**Website: <https://uwec.ly/hpcworkshop>**