

# Computational Techniques in Chemistry

By **Valentina Erastova**  
with Sarah Stewart,  
Audrey Ngambia,  
Tim Spankie,  
Chenfeng Zhang and Ryan  
Zhu

**Session 1: Introduction to Linux and command-line**

# What is computational chemistry?

---

Computational chemistry aims to simulate and predict molecular structures and properties using different kinds of calculations based on quantum and classical physics.

---

Computational techniques are **methods** and **tools** with which we perform these calculations.

# Why attend this course?



Computational techniques are integral part of modern research, contributing to scientific discovery.



Enable accurate **simulation** of chemical reactions and **prediction** of molecular properties, otherwise unattainable.



E.g., study of large protein complexes, biological membranes, molecular interactions, and extreme conditions.



Computational tools **accelerate** the development of new drugs, materials, and technologies.



It is now **essential for a modern chemist** to have basic skills and understanding of the computational techniques.



# What will I learn?



- **Practical Aspects:** Understand the practical aspects of molecular simulations.
- **Command-Line Interfaces:** Use basic command-line interfaces and operate on high-performance computing resources.
- **Computational Chemistry Software:** Use common computational chemistry packages to tackle real chemical problems.
- **Molecular Dynamics Simulations:** Prepare systems for molecular dynamics simulations and troubleshoot the set-up, simulations, and analysis steps.
- **Technique Limitations:** Understand the limitations of the computational chemistry techniques used.
- **Reporting:** Report the methodology and observations in a condensed written format.
- **Group Work:** Perform group work, encouraged and developed through the practicals.

# Examples of Computational Chemistry Careers



## Computational Chemist

... use of computational tools to solve chemical problems across various industries/topics

Superpowers 🦹 :

- Proficiency in computational tools
- Problem-solving skills
- Interdisciplinary collaboration

## Academic Research 📖

Conducting research in universities or research institutions, focusing on theoretical and computational methods to solve chemical problems.

Universities, Research Institutes

Skills:

- Strong analytical skills
- Programming
- Data Analysis
- Publication writing

## Pharmaceutical Industry 💊

Developing computational models to aid in drug discovery and development processes.

Pharmaceutical Companies, Biotech Firms

Skills:

- Knowledge of molecular modeling
- Bioinformatics
- Software development

## Material Science ✨

Using computational methods to design and discover new materials with desired properties.

Material Science Companies, Research Labs

Skills:

- Expertise in materials science
- Computational modeling
- Simulation techniques

## Environmental Science 🌍

Applying computational chemistry to understand and solve environmental issues, such as pollution and climate change.

Environmental Agencies, NGOs

Skills:

- Environmental modeling
- Data analysis
- Interdisciplinary knowledge

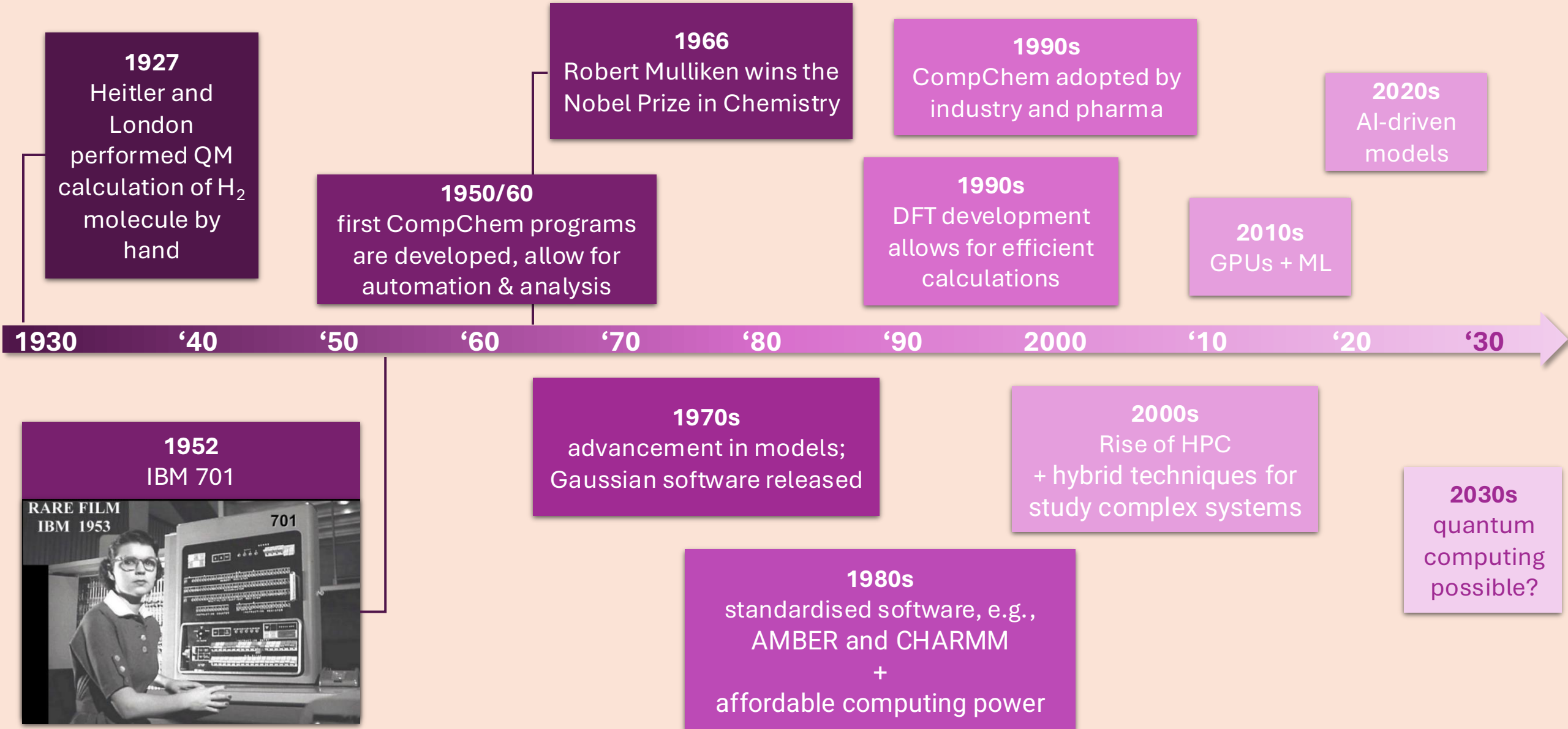
# Course organisation

	Monday/Tuesday	Thursday/Friday
Week 1	<b>Introduction to Linux and command-line</b>	
	Workshop	Drop-in
	Quiz 1 (5%) Deadline 27 <sup>th</sup> January	
Week 2	<b>Introduction to molecular dynamics simulations</b>	
	Workshop	Drop-in
	Quiz 2 (5%) Deadline 3 <sup>rd</sup> February	
Week 3	<b>Molecular simulation set up of system with an interface or a protein system</b>	
	Workshop	Drop-in
Week 4	Beginning of the <b>individual projects</b> (30% of the course mark)	
	Workshop	Drop-in
Week 5	Drop-in	
	<b>Project Submission</b> Monday 17 <sup>th</sup> February	



# Session 1: Introduction to Linux and command-line

# Historical Perspective

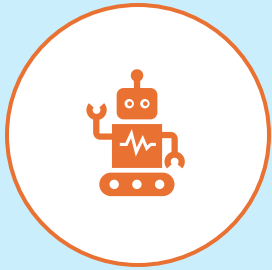




# Why the Unix Shell?



**shell** is a command-line interpreter or shell that provides a command-line user interface for Unix-like operating systems (that run our HPC).



Automates tasks



Streamlines data management and enables reproducibility



Gives access to enhanced computing power



Facilitates collaborations

# Why use High-Performance Computing?



## Handling Large-Scale Simulations

*simulate 100+k atom systems*



## Accelerating Computational Processes

*run time-intensive calculations*



## Enhancing Accuracy and Precision

*perform repeats and high accuracy calculations*



## Enabling Advanced Research Techniques

*access high-resource novel methods, e.g. QM or ML*



## Fostering Collaborative Research

*collaborate on large-scale projects across universities*

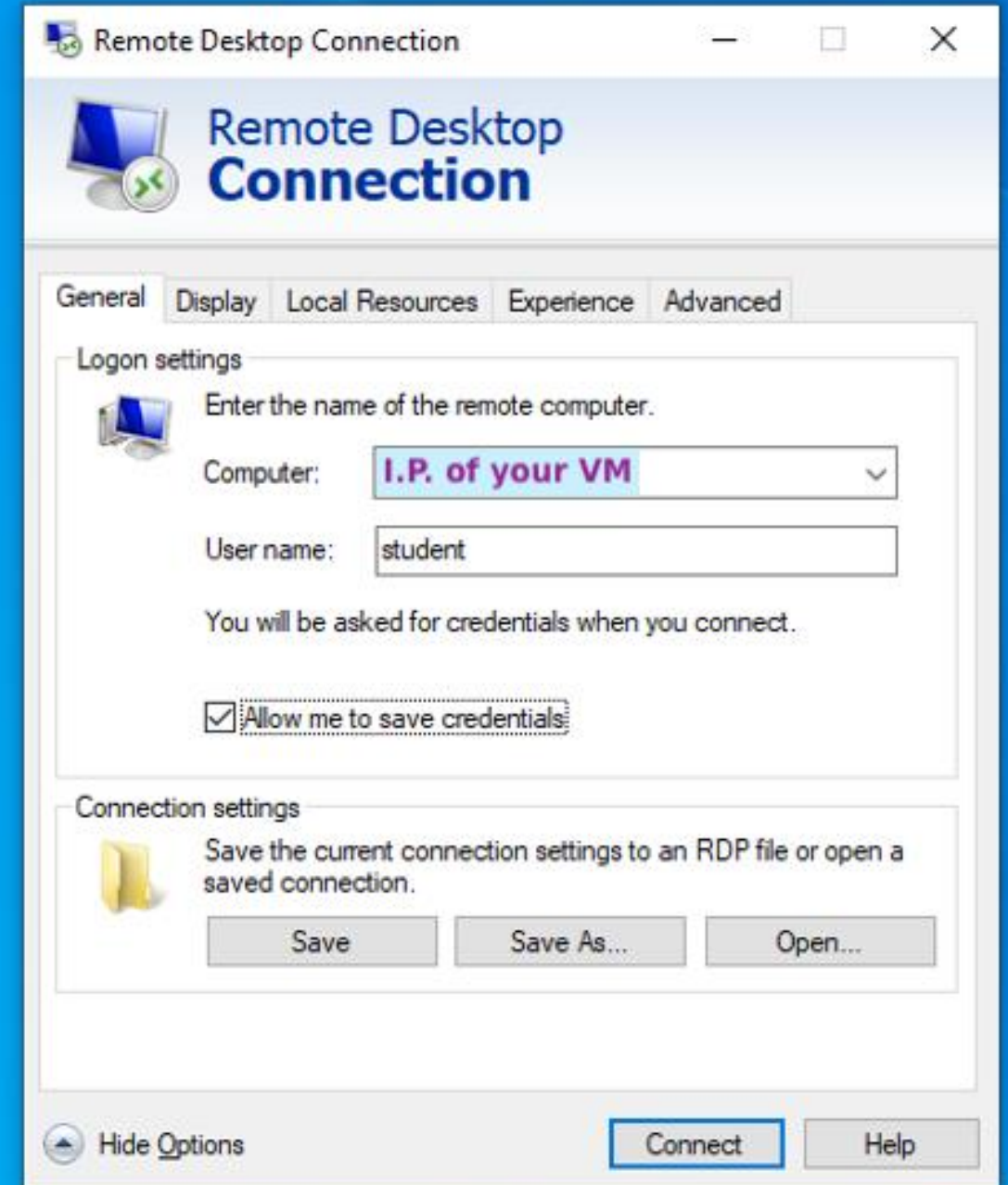
# Getting Started with Workshop



1

# Connecting to your Virtual Machine

1. Log into the computer in front of you
2. Open "**Remote Desktop Connection**" App
3. In the app click "*Show Options*"
4. Enter the **IP address of your VM**
5. Enter the **username** assigned to you, e.g. student
6. Tick the box for "*Allow me to save credentials*"

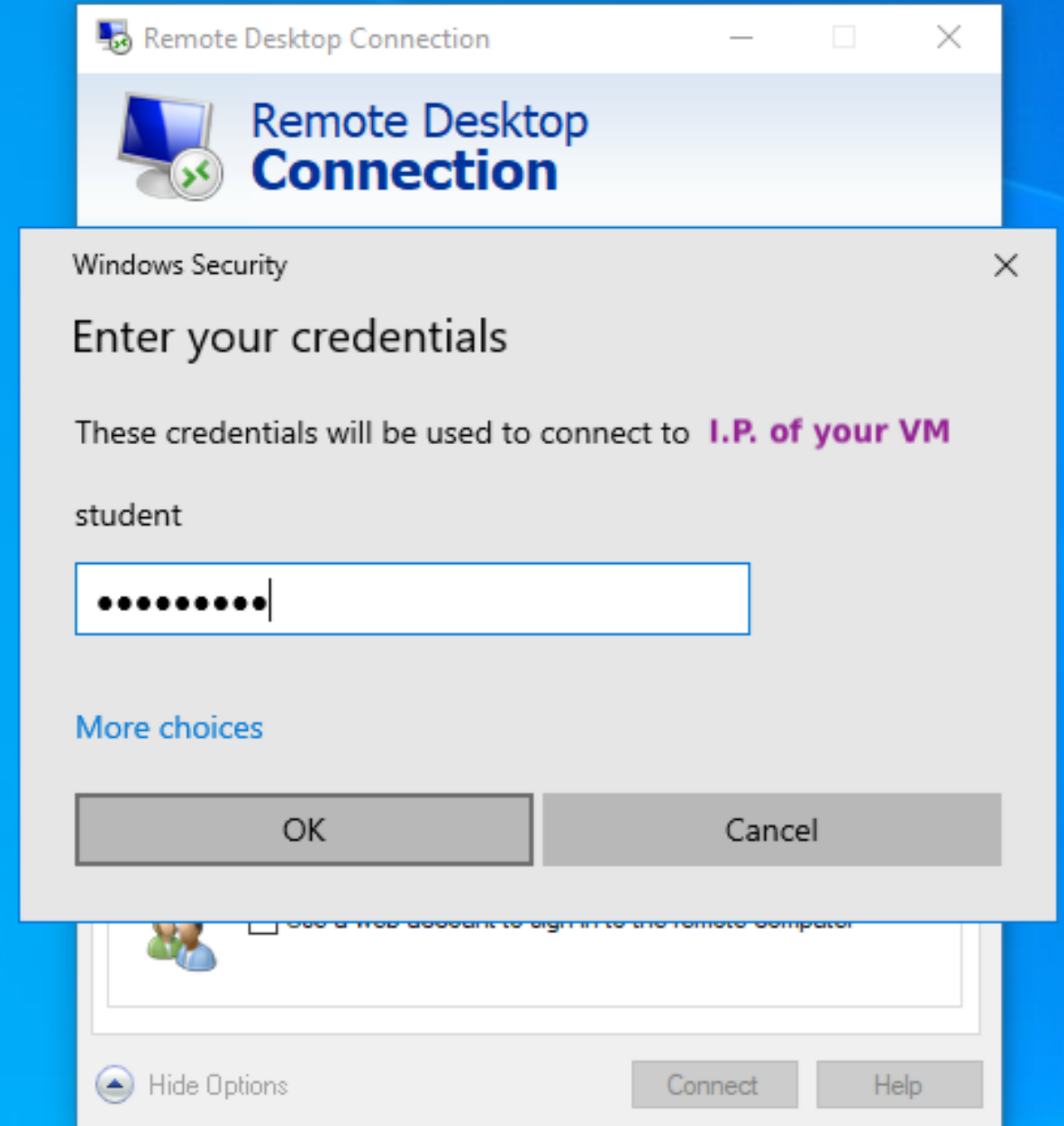




1

# Connecting to your Virtual Machine

7. Go to the "Advanced" tab
8. Click "Settings" under "Connect from anywhere"
9. Click "Do not use an RD Gateway server" and "OK"
10. Click "Connect"
11. When prompted to enter credentials, enter the **password**, e.g., dragonfly

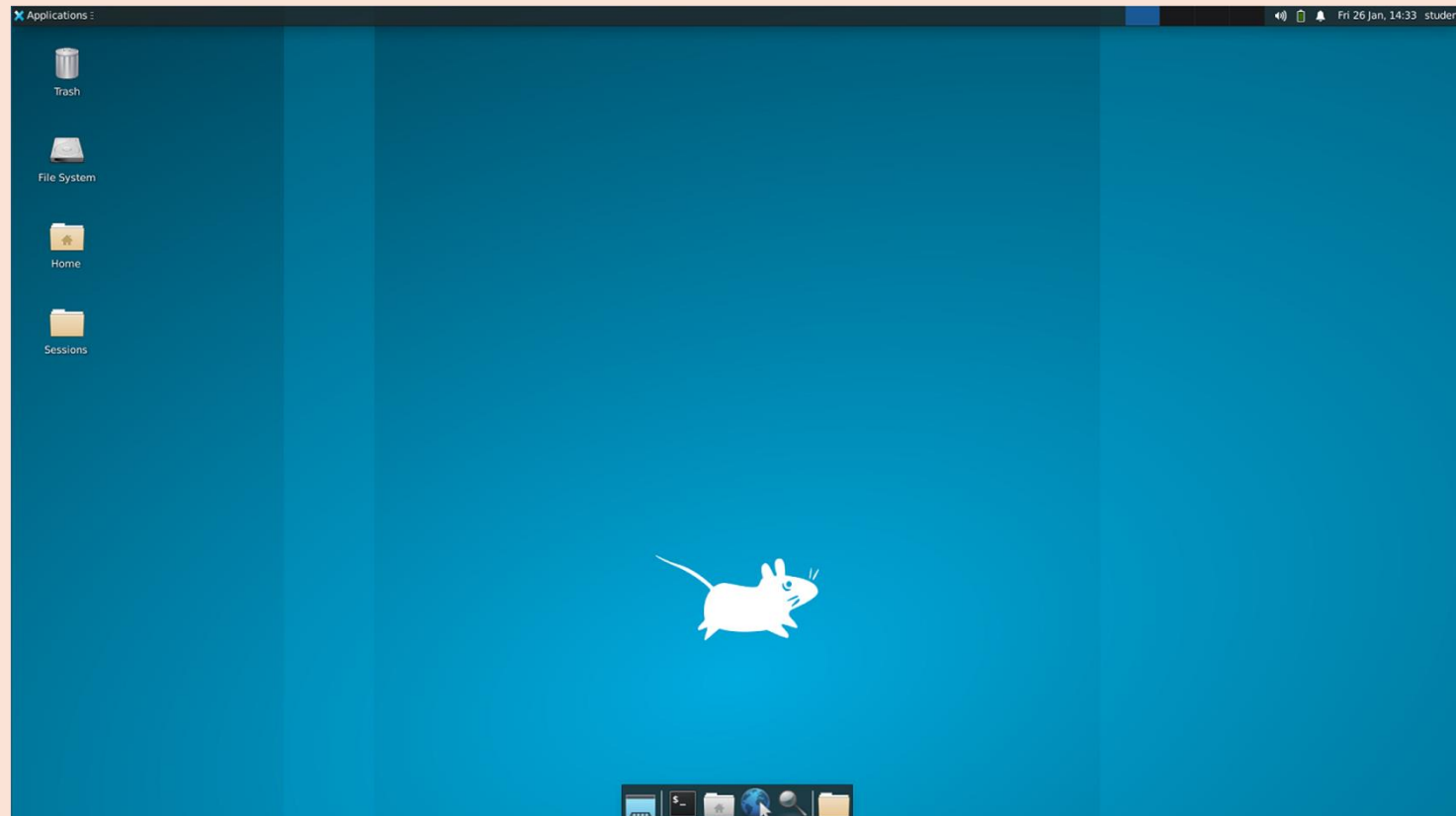


1

# Connecting to your Virtual Machine


## Success!

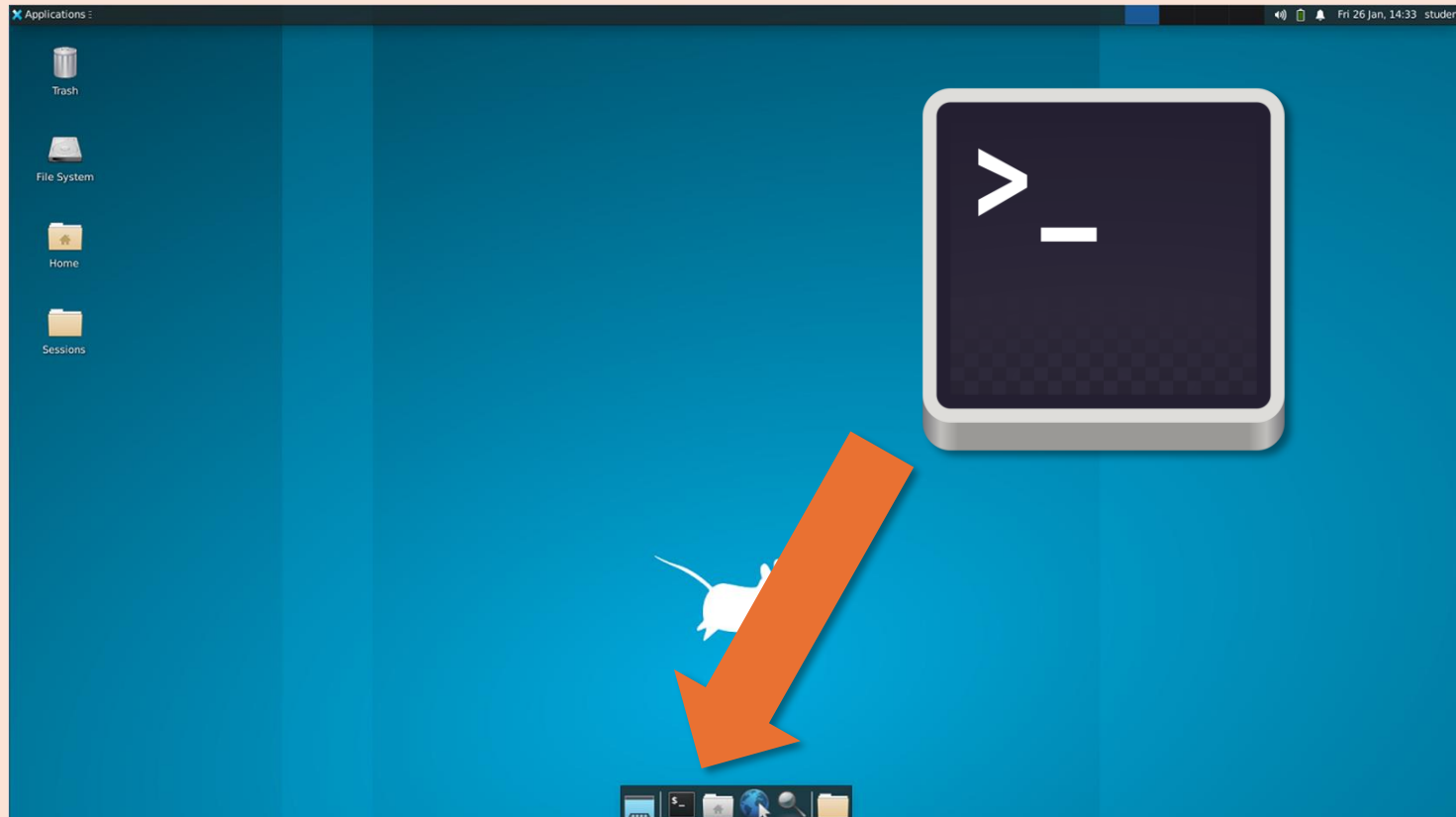
You may have an 'Authenticate' window pop up. Cancel it – it is not important.



2


# Starting with the Workshop

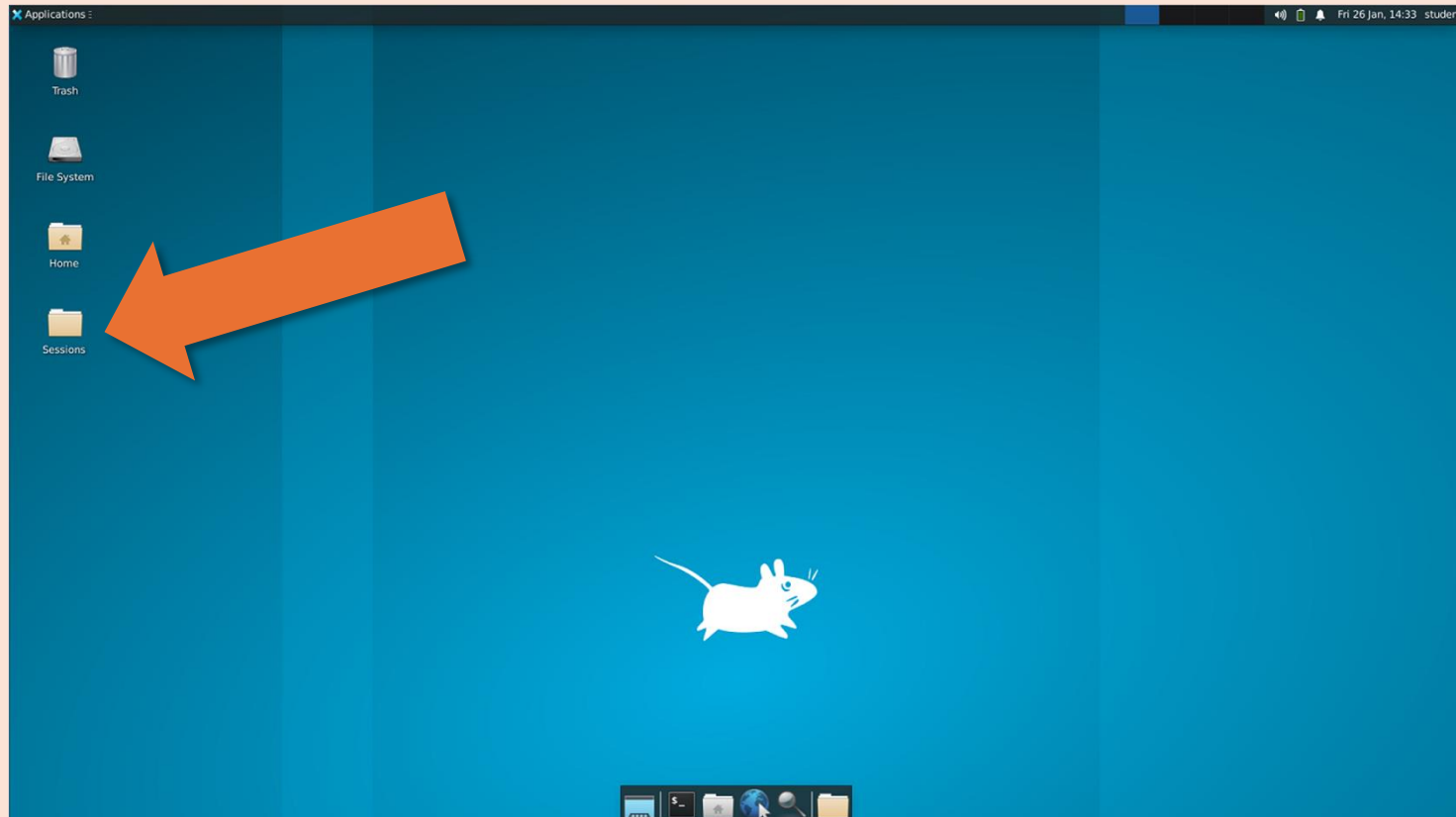
1. Click the  icon to load the **Terminal** app
2. The terminal window will open
3. You will be prompted for **UNN** and **password**  
– enter your university one.



2

# Starting with the Workshop

1. Click the  icon to load the **Terminal** app
2. The terminal window will open
3. You will be prompted for **UNN** and **password**  
– enter your university one.
3. Open '**Sessions**' folder and click on the '**Overview.html**'
4. Overview will load in the website browser
5. Click on '**Session 1**' to begin with today's workshop





3

Give us **feedback** at  
the end of each  
session!





# Questions?

Demonstrators are here to help!

Dr Valentina Erastova

[Valentina.Erastova@ed.ac.uk](mailto:Valentina.Erastova@ed.ac.uk)