

Computational Techniques in Chemistry

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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.

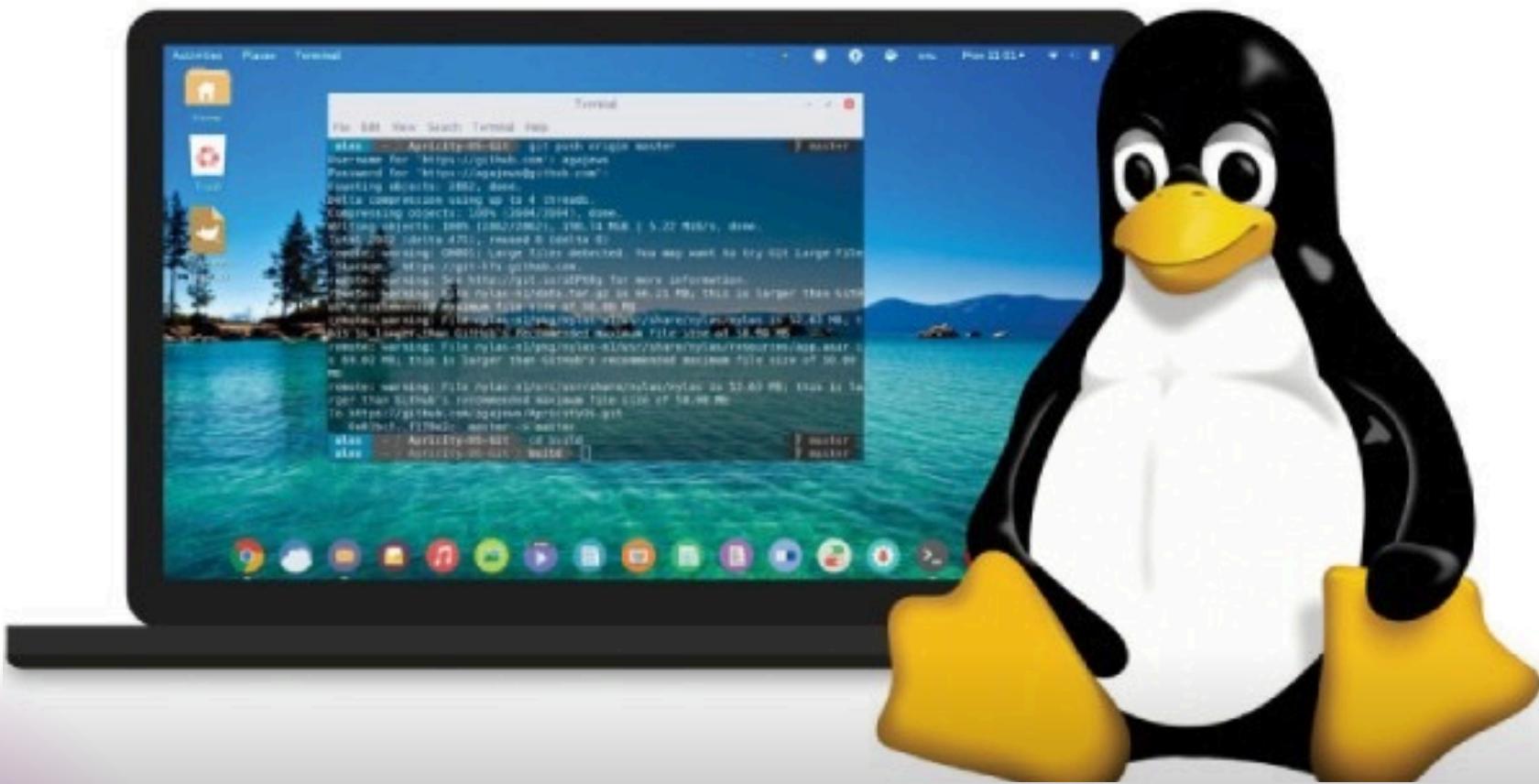
Environmental Agencies, NGOs

Skills:

- Environmental modeling
- Data analysis
- Interdisciplinary knowledge

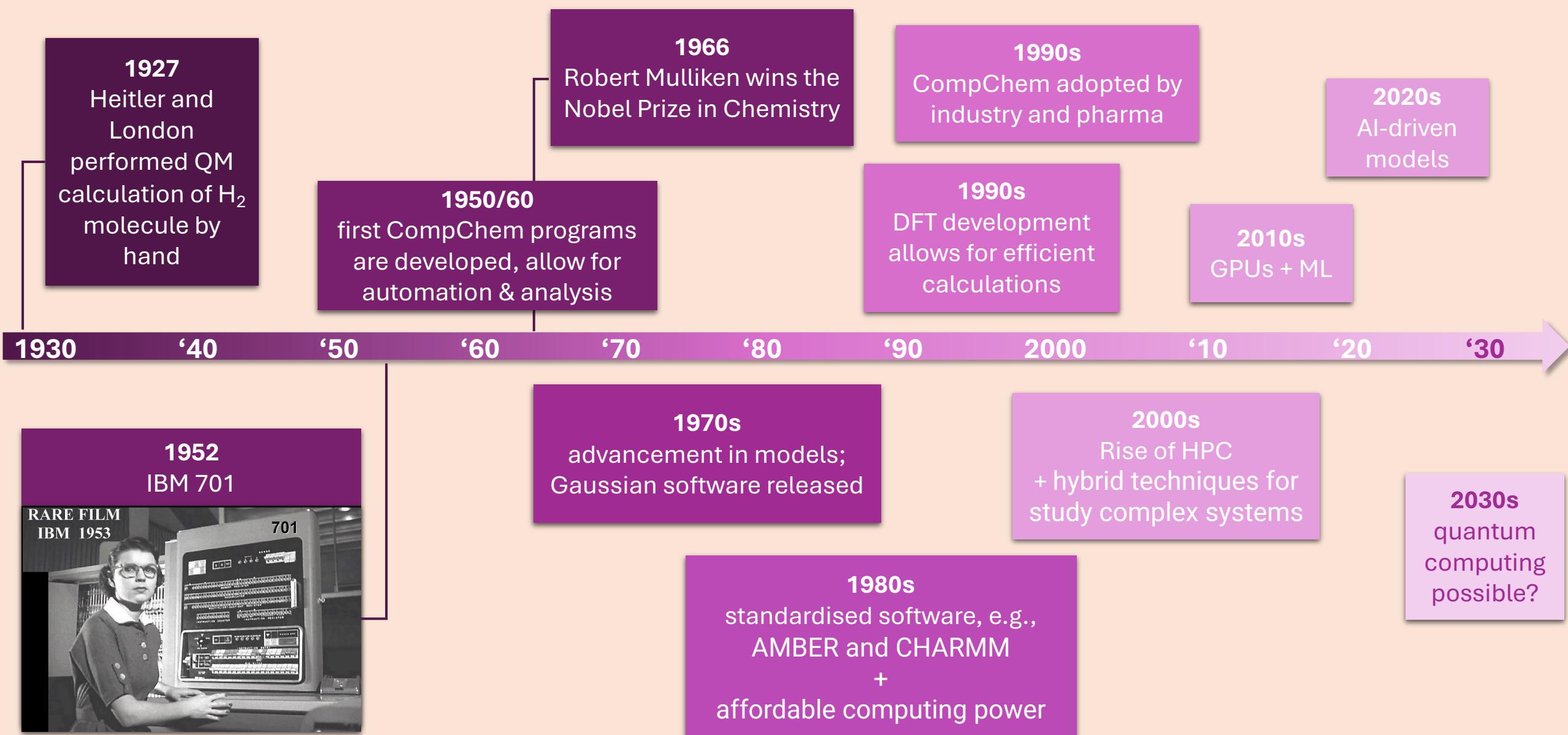
Course organisation

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



Session 1: Introduction to Linux and command-line

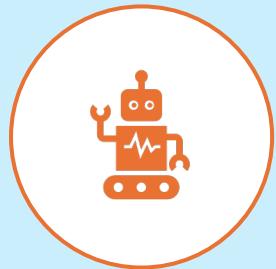
Historical Perspective



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

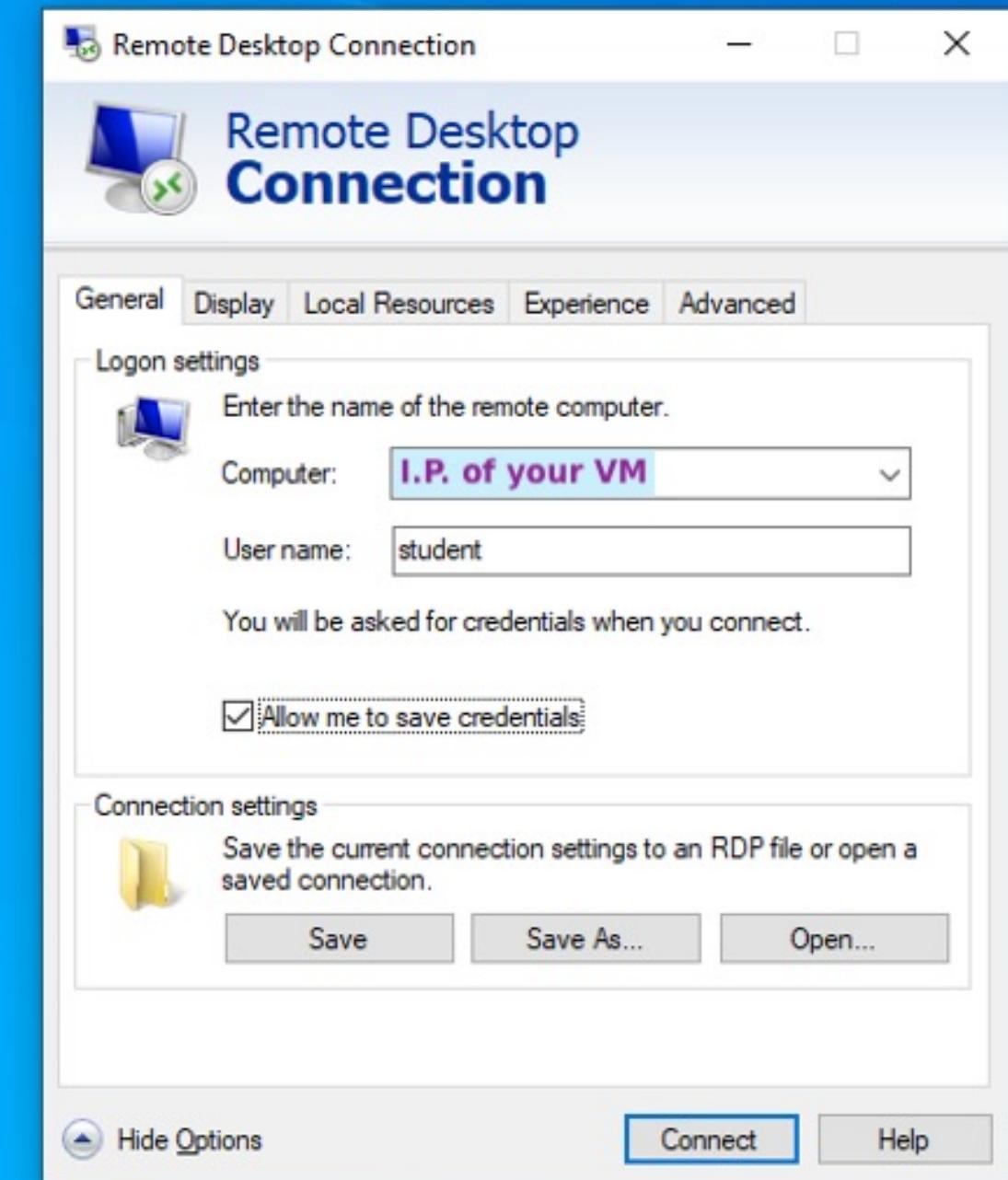
Getting Started with Workshop



1

Connecting to your Virtual Machine

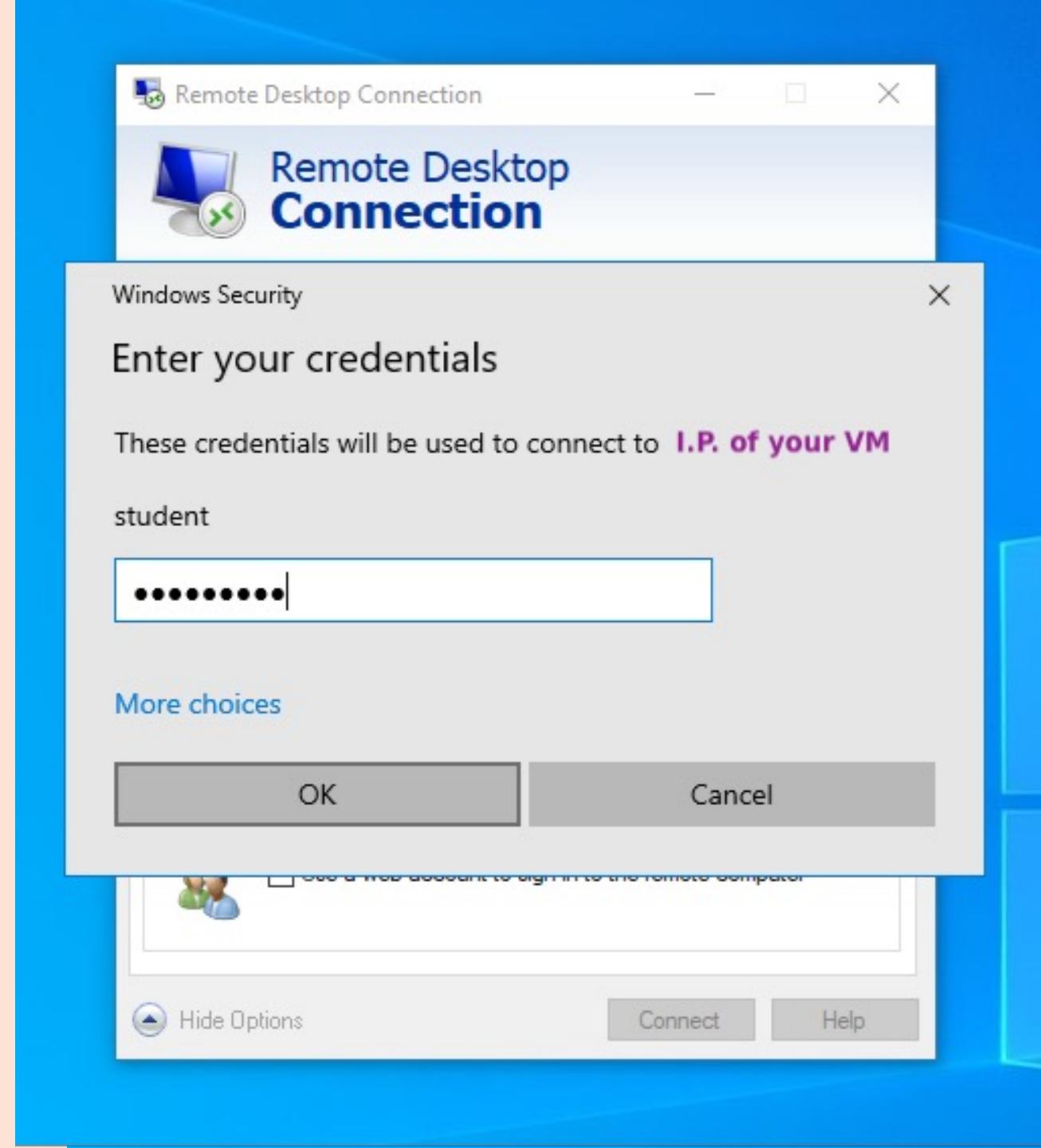
1. Log into the computer in front of you
2. Open "**Remote Desktop Connection**" App
3. In the app click "Show Options"
4. Enter the **IP address of your VM**
5. Enter the **username** assigned to you, e.g. **student**
6. Tick the box for "*Allow me to save credentials*"



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**

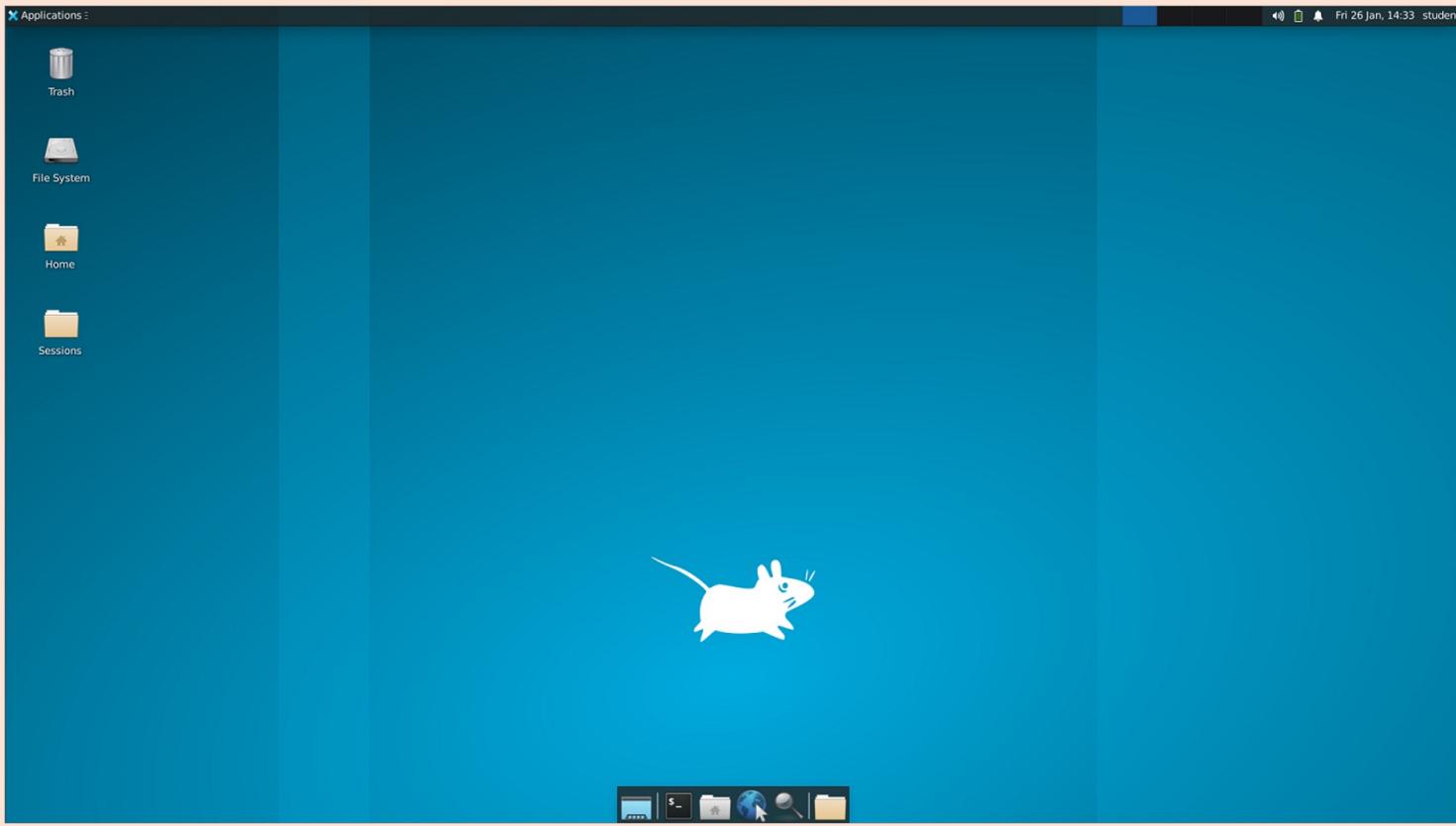


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Success!

Connecting to your Virtual Machine

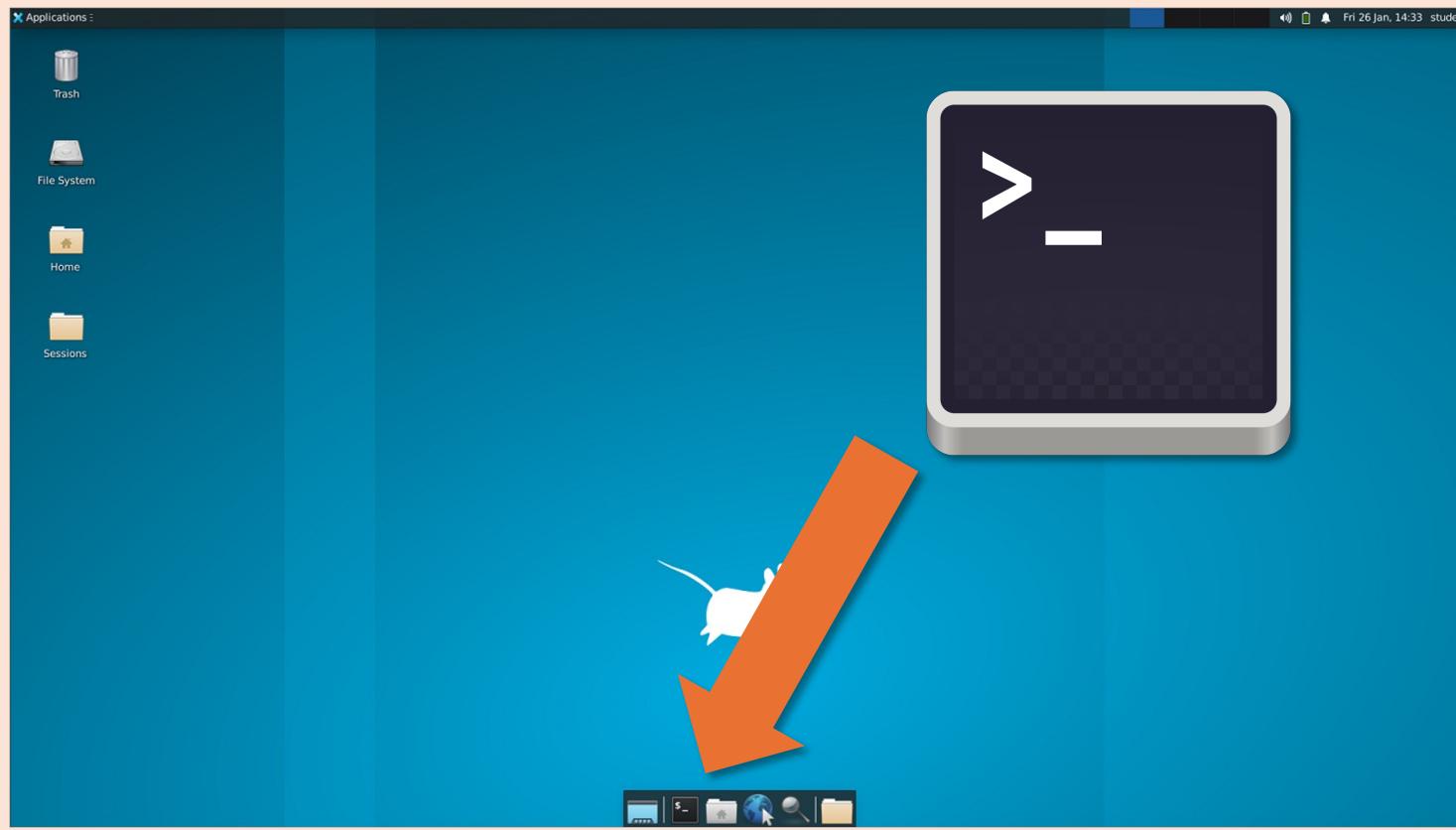
You may have an ‘Authenticate’ window pop up. Cancel it – it is not important.



2

Starting with the Workshop

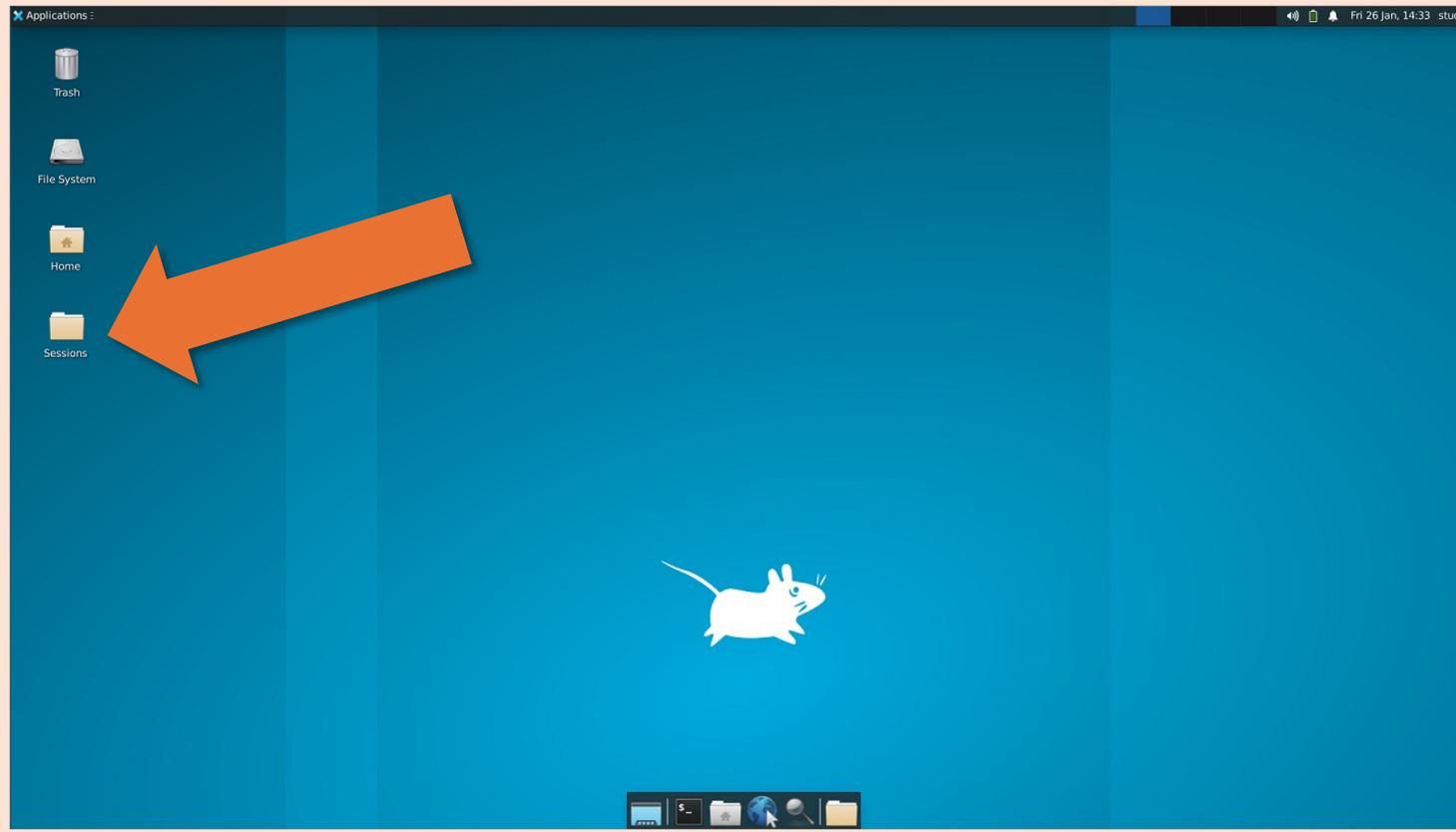
1. Click the **>_** icon to load the **Terminal** app
2. The terminal window will open
3. You will be prompted for **UNN** and **password**
– enter your university one.



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.
4. Open ‘**Sessions**’ folder and click on the ‘**Overview.html**’
5. Click on ‘**Session 1**’ to begin with today’s workshop



3

Plz give us **feedback**
at the end of each
session!

- 1 – go to wooclap.com
- 2 – event code **EUCRND**



Questions?

Demonstrators are here to help!

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