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Excited States and Nonadiabatic Dynamics
CyberTraining School/Workshop 2023

Alexey Akimov

University at Buffalo, SUNY

June 12, 2023

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General Workshop Goals

and

Overview of the CyberTraining Infrastructure

Objectives and Agenda

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CyberTraining: Pilot: Modeling Excited State Dynamics in Solar Energy Materials

Workshop Objectives

- Get **familiar with a variety of software packages** relevant to modeling of excited states and nonadiabatic dynamics
- Get an overview of **theoretical background** for corresponding computational methods
- Get a **practical experience** with these tools and packages

Keywords and topics:

- nonadiabatic dynamics
- excited states
- quantum dynamics
- quantum-classical methods
- charge transfer
- excitation energy transfer
- trajectory surface hopping
- coupled trajectories
- exact factorization
- TD-DFT, CASSCF, GW/BSE
- algorithms and methods
- software, programming, Python
- best practices, Git, GitHub

This year

- Libra (Akimov)
- Quantics/MCTDH (Worth)
- GAMESS (Filatov)
- NWChem (Govind)
- TT-SOFT, TT-Chebyshev (Soley)

2022 (in person/virtual)

- pyUNIxMD (Min)
- CT-MQC (Ibele)
- SHARC (Mai)
- SHARC/COBRAMM (Avagliano)
- OpenMolcas (Mai, Avagliano)
- ORCA (Mai)
- Hefei-NAMD (Zhao, Chu)
- Quantum Espresso (Zhao, Chu)
- BerkeleyGW and paratec (Zhang)
- DynEMol (Rego)
- Libra (Akimov)
- DFTB+ (Shakiba)
- CP2K (Shakiba)
- TBD (Kilin)

2021 (virtual)

- Libra (Akimov)
- NEXMD (Tretiak)
- Newton-X (Barbatti)
- nano-qmflows (Infante, Zapata)
- CAT, auto-FOX (Infante, Zapata)
- COLUMBUS (Lischka)
- DFTB+
- CP2K
- Quantum Espresso
- ErgoSCF

The Plan & Resource

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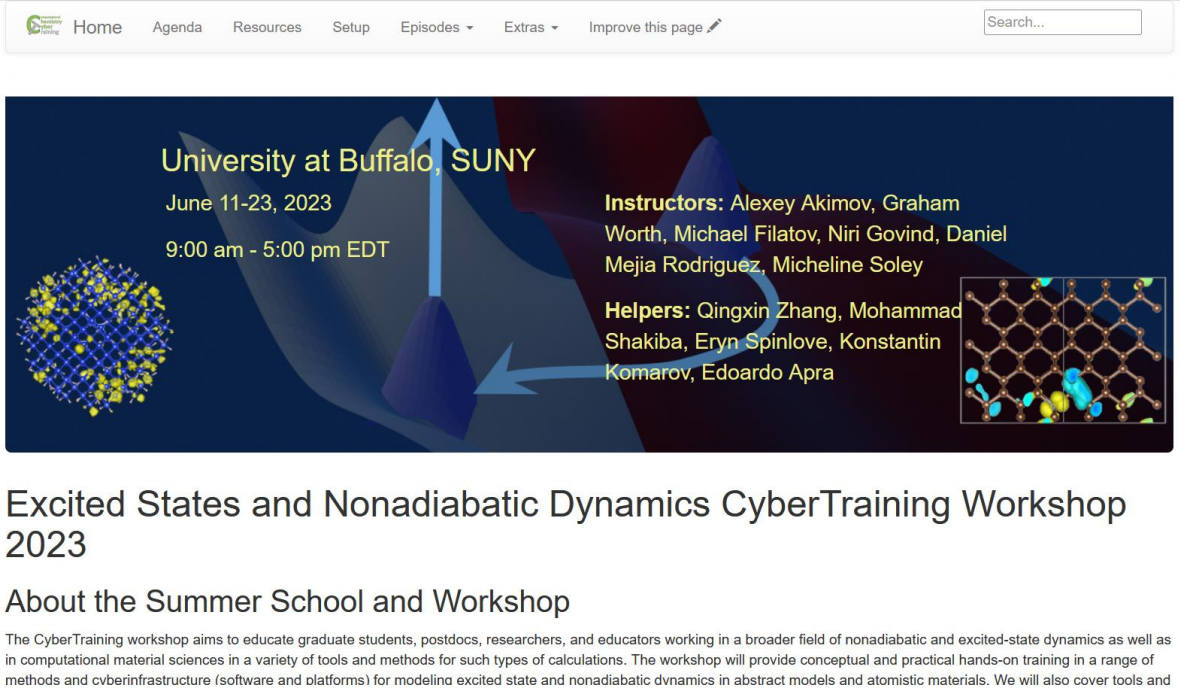
All the details are here:

https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2023



Join Slack:

- Members can invite new members
- Private and public channels, direct (private) messages, conversations
- Any time, no strings attached

https://join.slack.com/t/quantumdynamicshub/shared_invite/zt-mjbhjssx-GGhsbYHxeBMvhmumK_j7LA

VPN and Accounts:

- 2-factor authentication
- submit a ticket: https://ubccr.freshdesk.com/support/home

Topics and Instructors

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June 12, 2023 (Day 2), **Monday**	**Morning, 9 am - noon** • Worshop Kick Off: goals, logistics, details. Overview of the CCR CyberInfrastructure (30 min) • Working with Git and GitHub. Theory and Hands on (60 min) • General overview of Libra software (Lecture)(30 min) • General overview of Libra software (Hands on)(60 min) **Noon - 1:30 pm** Lunch break **Afternoon, 1:30 pm - 5:00 pm** • Theory of adiabatic and nonadiabatic dynamics. Lecture (120 min) • TSH and Ehrenfest dynamics with model Hamiltonians in Libra. Hands on (50 min) • TSH and Ehrenfest dynamics with model Hamiltonians in Libra. Hands on (50 min)	Alexey Akimov, Qingxin Zhang, Mohammad Shakiba
June 13, 2023 (Day 3), Tuesday	**Morning, 9 am - noon** • Overview of the NBRA workflow. step4 (dynamics) within the NBRA settings. Lecture/HandsOn (30 min) • Computing NACs in the MO basis with DFTB+ (30 min) • Mapping single-particle properties to the Slater-determinants picture (30 min) • Complete example with DFTB+ (60 min) • Interfacing Libra with external codes (30 min) **Noon - 1:30 pm** Lunch break **Afternoon, 1:30 pm - 5:00 pm** • NA-MD in finite and condensed matter systems with xTB and TD-DFT with Libra/CP2k code. Lecture and Hands on	Alexey Akimov, Qingxin Zhang, Mohammad Shakiba

Libra

https://github.com/Quantum-Dynamics-Hub/libra-code

https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2023/_episo des/03-libra

https://github.com/compchem-cybertraining/Tutorials_Libra

https://github.com/compchem-cybertraining/Tutorials_DFTB_plus

https://github.com/compchem-cybertraining/Tutorials_CP2K

Alexey Akimov

Mohammad Shakiba

Qingxin Zhang

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June 14, 2023 (Day 4), Wednesday	**Morning, 9 am - noon** • Theory and hands on with Quantics and MCTDH **Noon - 1:30 pm** Lunch break **Afternoon, 1:30 pm - 5:00 pm** • Theory and hands on with Quantics and MCTDH	Graham Worth, Eryn Spinlove
June 15, 2023 (Day 5), Thursday	**Morning, 9 am - noon** • Theory and hands on with Quantics and MCTDH **Noon - 1:30 pm** Lunch break **Afternoon, 1:30 pm - 5:00 pm** • Theory and hands on with Quantics and MCTDH	Graham Worth, Eryn Spinlove

Quantics

http://www2.chem.ucl.ac.uk/quantics/

https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2023/_episodes/04-quantics

https://github.com/compchem-cybertraining/Tutorials_Quantics

Graham Worth

Eryn Spinlove

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June 16, 2023 (Day 6), Friday	**Morning, 9 am - noon** • Theory: Introduction in ensemble DFT and basic aspects of REKS method for ground electronic states **Noon - 1:30 pm** Lunch break **Afternoon, 1:30 pm - 5:00 pm** • Hands on: REKS implementation in GAMESS-US; Demos and practical exercises with REKS method for strongly correlated molecular ground states.	Michael Filatov, Konstantin Komarov
June 17, 2023 (Day 7), Saturday	On your own. Projects time	
June 18, 2023 (Day 8), Sunday	On your own. Projects time	
June 19, 2023 (Day 9), **Monday**	**Morning, 9 am - noon** • Theory: Ensemble DFT for excited states and its implementation in state-averaged REKS methodology **Noon - 1:30 pm** Lunch break **Afternoon, 1:30 pm - 5:00 pm** • Hands on: Practical exercises with GAMESS-US and NAMD simulations with GAMESS/pyUNI-xMD package	Michael Filatov, Konstantin Komarov

GAMESS US

https://www.msg.chem.iastate.edu/gamess/

https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2023/_episodes/05-gamess

https://github.com/compchem-cybertraining/Tutorials_GAMESS

Michael Filatov (Gulak)

Konstantin Komarov (remotely)

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June 20, 2023 (Day 10), Tuesday	**Morning, 9 am - noon** • Theory and hands on with NWChem **Noon - 1:30 pm** Lunch break **Afternoon, 1:30 pm - 5:00 pm** • Theory and hands on with NWChem	Daniel Mejia Rodriguez, Edoardo Apra, Niri Govind
June 21, 2023 (Day 11), Wednesday	**Morning, 9 am - noon** • Theory and hands on with NWChem **Noon - 1:30 pm** Lunch break **Afternoon, 1:30 pm - 5:00 pm** • Theory and hands on with NWChem	Daniel Mejia Rodriguez, Edoardo Apra, Niri Govind

NWChem

https://nwchemgit.github.io

Daniel Mejia-Rodriguez

Niri Govind (remotely)

Edoardo Apra (remotely)

https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2023/_episodes/06-nwchem

https://github.com/compchem-cybertraining/Tutorials_NWChem

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June 22, 2023 (Day 12), Thursday	**Morning, 9 am - noon** • Theory of quantum dynamics with TT-SOFT and TT-Chebyshev, IPA optimization. **Noon - 1:30 pm** Lunch break **Afternoon, 1:30 pm - 5:00 pm** • Hands on with TT-SOFT and TT-Chebyshev, IPA optimization.	Micheline Soley

TT-SOFT and TT-Chebyshev

https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2023/_episodes/07-ttsoft

https://github.com/compchem-cybertraining/Tutorials_NWChem

Micheline Soley

Please Introduce Yourself

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- Name, position, affiliation, research group
- Research interests and expertise
- Anything else you would like to share with us

More Resources

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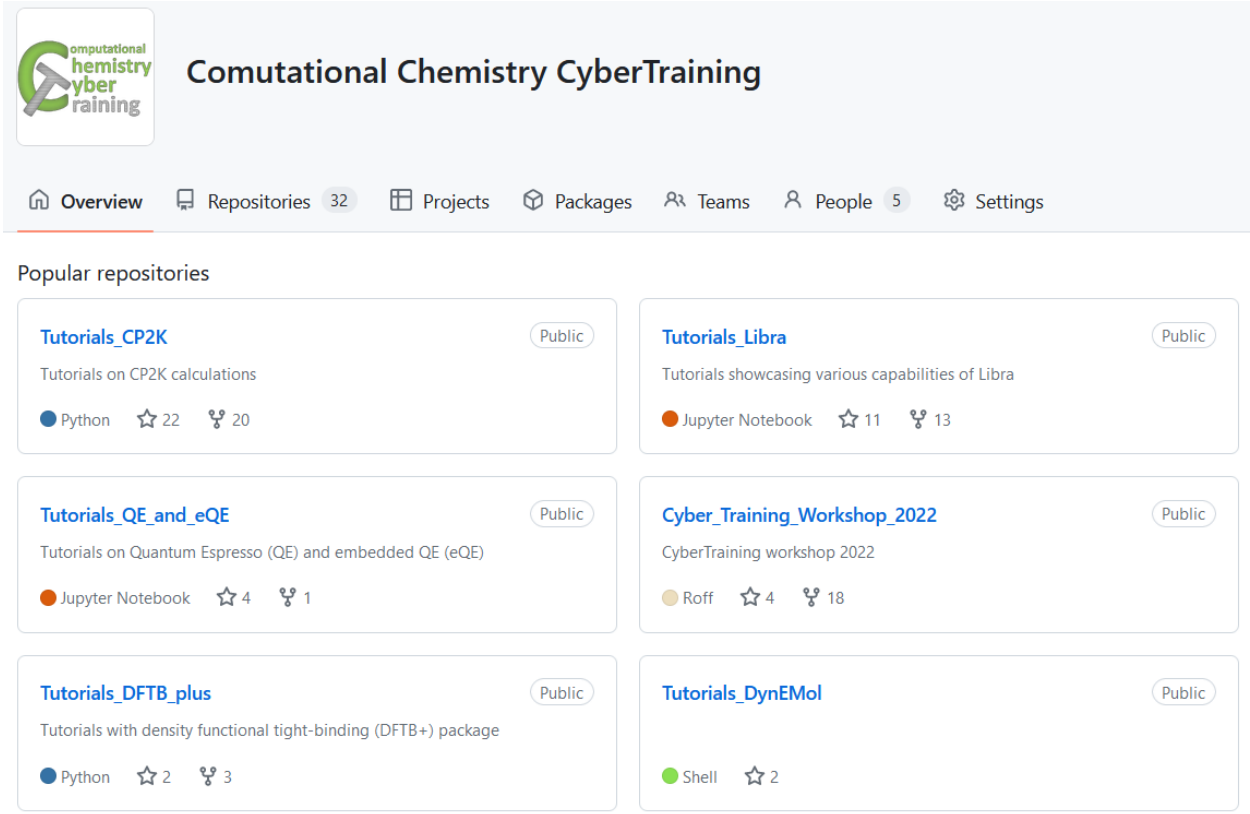
Codes: https://github.com/Quantum-Dynamics-Hub
Training: https://github.com/compchem-cybertraining

Quantum Dynamics Hub: https://quantum-dynamics-hub.github.io/

Summer 2021 workshop: https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2021/

Libra Winter school: https://compchem-cybertraining.github.io/Libra_Winter_School_2022/

Summer 2022 workshop: https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2022/



Summer 2023 (This!) workshop: https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2023/

Daily Schedule

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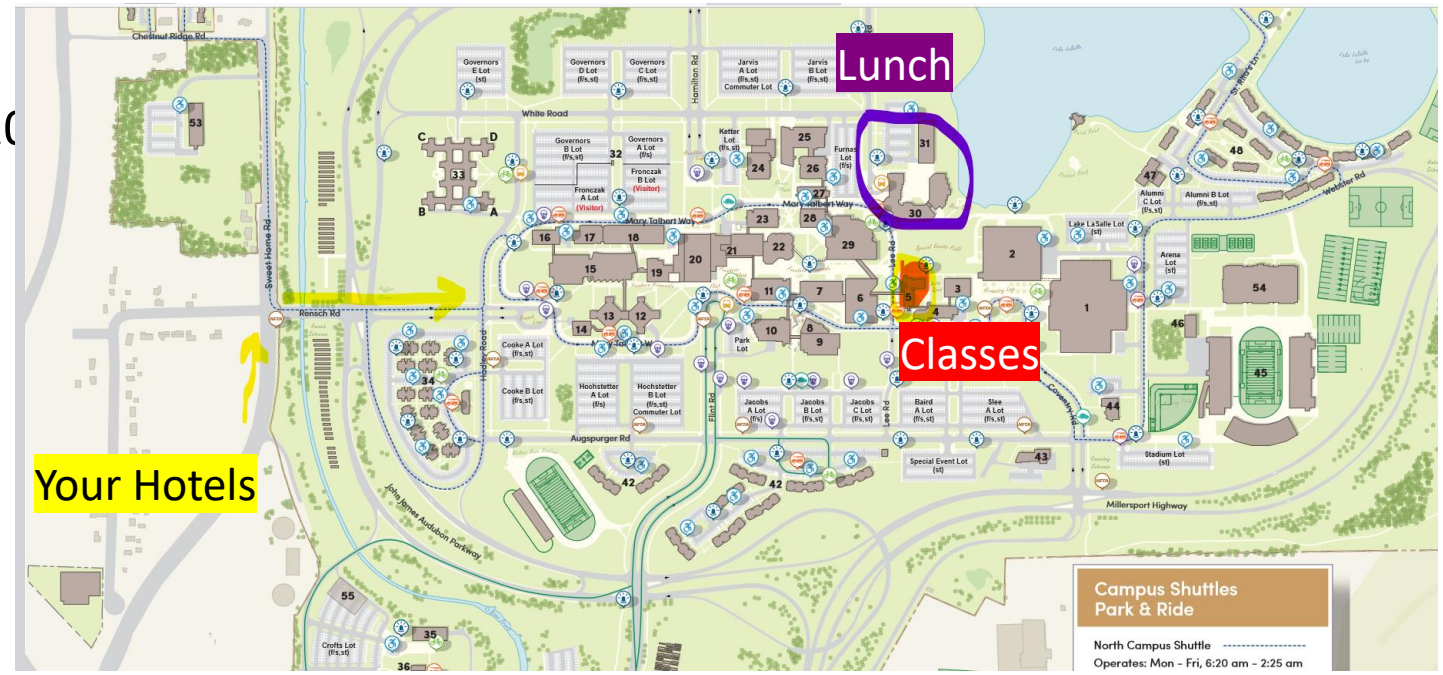
Daily

- Breakfast = hotel
- 9:00 am – 12:00 pm: Morning session (Recording)
- 12:00 – 1:30 pm Working lunch/rest – on your own at “Commons”, rest, discuss, collaborate
- 1:30 pm – 5:00 pm: Afternoon session (Recording)
- After 5:00 pm: collaborations/on your own, dinner on your own

Location

- Classes are @: June 12 – 22 Clemens 12(

Campus Map:
https://emergency.buffalo.edu/content/dam/www/parking/North%20Campus%20Parking%20Map%2011x17.pdfhttps://emergency.buffalo.edu/content/dam/www/parking/North%20Campus%20Parking%20Map%2011x17.pdf



Logistic

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- We cover your hotel stay (except for the local folks). Stipends also cover the rest of expenses, please keep your receipts just in case. Let me know your flight expenses via the Google form provided on Slack channel.

- Travel for the US participants to a reasonable amount, partially the international participants (as the funds allow), except for local/UB-affiliated folks.

- Paperwork: All trainees will need to fill in the RF Participation Stipend form and one of the other two forms: W-9 - for the US residents and W-8BEN for the non-residents. The forms are distributed to you **via Slack** – please **DON't sent them back via e-mail** – upload to the form provided or via Slack.

- A lot of paperwork later – likely it'll be just me handling most of the stuff

- Prizes: $300 (1 first prize), $200 (3 second prizes), $100 (5 first prizes) – the project competition. Online and in-person participants are eligible. UB-affiliated participants are eligible too.

- Reimbursement/honoraria to the instructors – a separate paperwork. Will send you instructions via the Instructors Channel on Slack.

Course Project

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Project rules

https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2023/CODE_OF_CONDUCT.html

- Consist of: a) short written report, b) presentation at the last day of workshop; c) set of input/output files deposited on the GitHub repository
- Should actively involve one of the packages discussed over the workshop period
- Preferably not something you have an extensive experience with
- Doesn't have to be a full-scale research project, but can be a step towards this direction
- Projects completed using local or home institution resources are eligible
- Can be an application or a coding project
- The consistency in your course work during this school will contribute to your chances to win the awards
- The awards decisions will be made based on the committee evaluation. The awards will be: 1 first prize ($300), 3 second

- Submit your project via GitHub by June 30
- Oral presentation – tentatively July 1-2, via Zoom

Check out the past years' projects:

https://github.com/compchem-cybertraining/Cyber_Training_Workshop_2021/tree/gh-pages/course_work
https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2021/_episodes/13-projects

https://github.com/compchem-cybertraining/Cyber_Training_Workshop_2022/tree/gh-pages/course_work
https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2022/_episodes/15-projects

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Getting Started on UB CCR

Accessing UB Computing Resources

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Before the Workshop

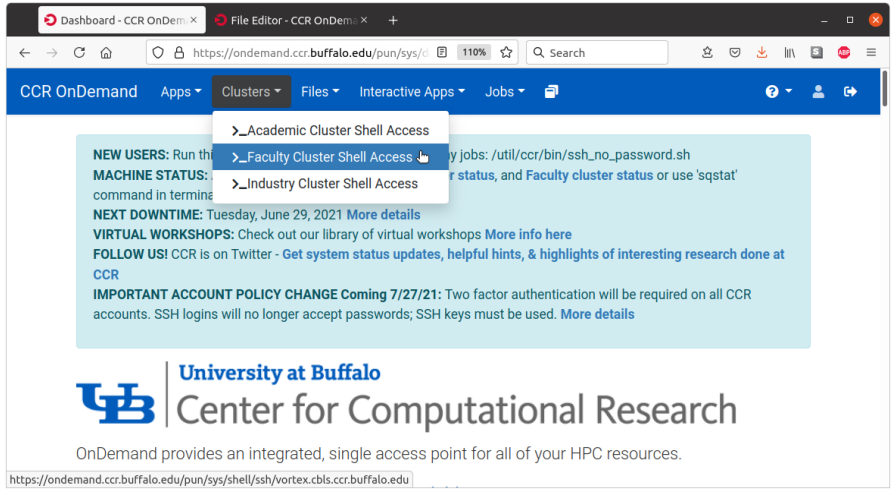
https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2023/setup.html

https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2023/_episodes/01-introduction

OnDemand (not Firefox, use Chrome)

On campus – nothing special;
Off-campus – use UB VPN

https://ondemand.ccr.buffalo.edu/

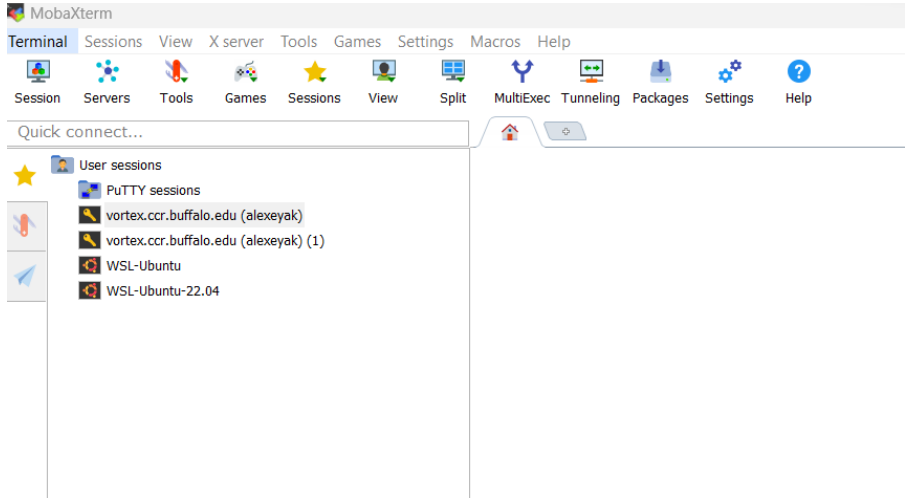


Moba Xterm

Generate the SSH public/private key.

- Use Moba Tools -> MobaKeyGen
- Coordinate it with your UB credentials

https://docs.ccr.buffalo.edu/en/latest/portals/idm/



Accessing UB Computing Resources

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Your **.bashrc** file (in your home directory)

```
# .bashrc

# User specific aliases and functions

# Source global definitions
if [ -f /etc/bashrc ]; then
        . /etc/bashrc
fi
module use /projects/academic/cyberwksp21/Modules
eval "$(/projects/academic/cyberwksp21/SOFTWARE/Conda/bin/conda shell.bash hook)"
```

- Restart terminal or `source .bashrc`
- For terminal-based operations: Activate conda environment: `conda activate libra2`
- For Jupyter – just launch it

Projects directory: /projects/academic/cyberwksp21 - slower, smaller, but permanent
Scratch space: /panasas/scratch/grp-cyberwksp21 - faster, larger, but temporarily (unused files are cleaned up every 1 or 2 weeks)

Using Jupyter Notebooks

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https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2023/_episodes/01-introduction