

Excited States and Nonadiabatic Dynamics *CyberTraining School/Workshop 2023*

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University at Buffalo, SUNY

June 12, 2023

General Workshop Goals
and
Overview of the CyberTraining Infrastructure

Objectives and Agenda

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

All the details are here:

[https://compchem-cybertraining.github.io/Cyber Training Workshop 2023](https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2023)

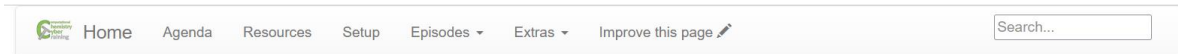
Join Slack:

- 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>



Excited States and Nonadiabatic Dynamics CyberTraining Workshop 2023

About the Summer School and Workshop

The CyberTraining workshop aims to educate graduate students, postdocs, researchers, and educators working in a broader field of nonadiabatic and excited-state dynamics as well as in computational material sciences in a variety of tools and methods for such types of calculations. The workshop will provide conceptual and practical hands-on training in a range of methods and cyberinfrastructure (software and platforms) for modeling excited state and nonadiabatic dynamics in abstract models and atomistic materials. We will also cover tools and

Topics and Instructors

June 12, 2023 (Day 2), **Monday**

Morning, 9 am - noon

- Workshop 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/_episodes/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

Topics and Instructors

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

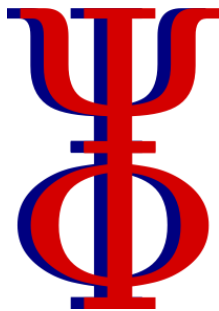
- Theory and hands on with Quantics and MCTDH

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

Topics and Instructors

June 16, 2023 (Day 6), Friday	Morning, 9 am - noon <ul style="list-style-type: none">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 <ul style="list-style-type: none">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 <ul style="list-style-type: none">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 <ul style="list-style-type: none">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)

Topics and Instructors

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://www.nwchem-sw.org/>



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

Topics and Instructors

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

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

More Resources

Codes: <https://github.com/Quantum-Dynamics-Hub>

Training: <https://github.com/compchem-cybertraining>

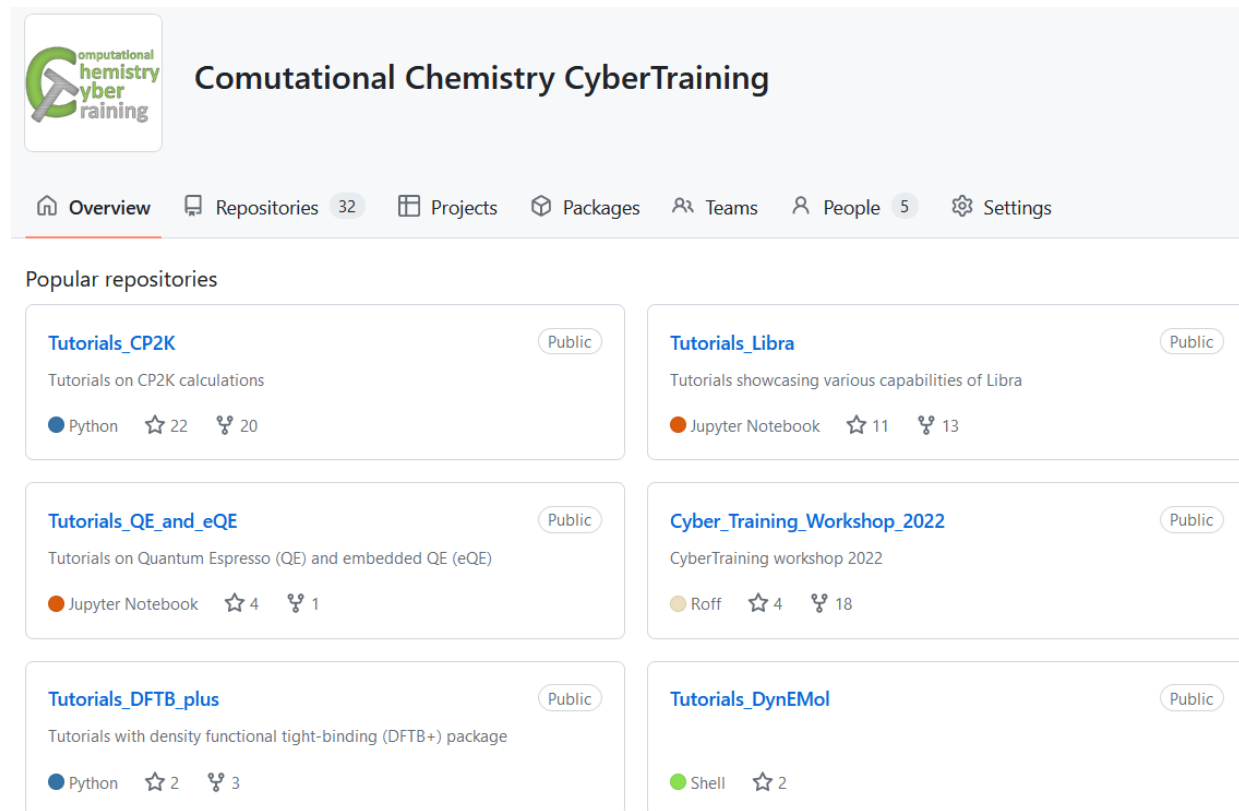
Quantum Dynamics Hub: <https://quantum-dynamics-hub.github.io/>

Summer 2021 workshop: [https://compchem-cybertraining.github.io/Cyber Training Workshop 2021/](https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2021/)

Libra Winter school: [https://compchem-cybertraining.github.io/Libra Winter School 2022/](https://compchem-cybertraining.github.io/Libra_Winter_School_2022/)

Summer 2022 workshop: [https://compchem-cybertraining.github.io/Cyber Training Workshop 2022/](https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2022/)

Summer 2023 (This!) workshop: [https://compchem-cybertraining.github.io/Cyber Training Workshop 2023/](https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2023/)



The screenshot shows the GitHub repository page for "Computational Chemistry CyberTraining". The repository is public and has 32 repositories, 0 projects, 0 packages, 0 teams, 5 people, and 0 settings. The "Popular repositories" section lists six repositories:

Repository Name	Description	Language	Stars	Forks	Public
Tutorials_CP2K	Tutorials on CP2K calculations	Python	22	20	Yes
Tutorials_Libra	Tutorials showcasing various capabilities of Libra	Jupyter Notebook	11	13	Yes
Tutorials_QE_and_eQE	Tutorials on Quantum Espresso (QE) and embedded QE (eQE)	Jupyter Notebook	4	1	Yes
Cyber_Training_Workshop_2022	CyberTraining workshop 2022	Roff	4	18	Yes
Tutorials_DFTB_plus	Tutorials with density functional tight-binding (DFTB+) package	Python	2	3	Yes
Tutorials_DynEMol		Shell	2		Yes

Daily Schedule

Daily

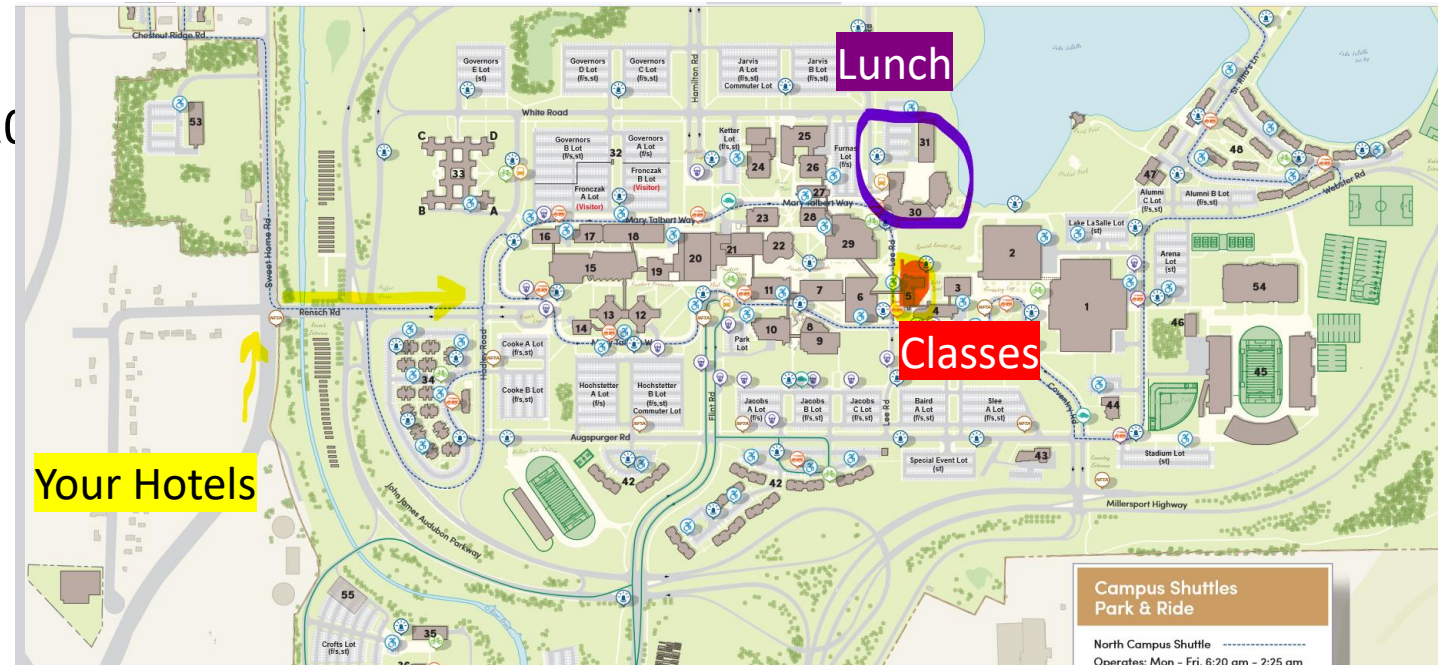
- Breakfast = hotel
- 9:00 am – 12:00 pm: Morning session (Recording)
- 12:00 – 1:30 pm Working lunch/rest – on your own at “Commons”, rest, discuss, collaborate
- 1:30 pm – 5:00 pm: Afternoon session (Recording)
- After 5:00 pm: collaborations/on your own, dinner on your own

Location

- Classes are @: June 12 – 22 Clemens 120

Campus Map:

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



- 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

Project rules

[https://compchem-cybertraining.github.io/Cyber Training Workshop 2023/CODE OF CONDUCT.html](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://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://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://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](https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2022/episodes/15-projects)

Getting Started on UB CCR

Accessing UB Computing Resources

Before the Workshop

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

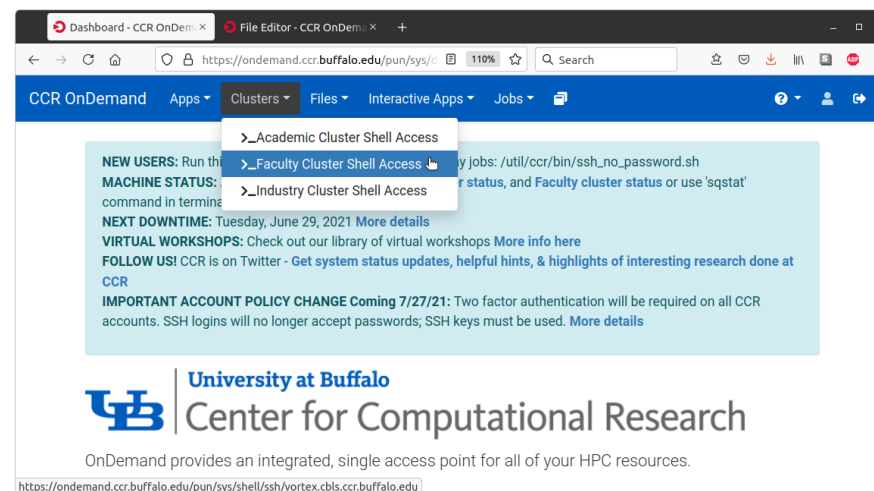
https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2023/_episodes/01-introduction

OnDemand (not Firefox, use Chrome)

On campus – nothing special;

Off-campus – use UB VPN

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

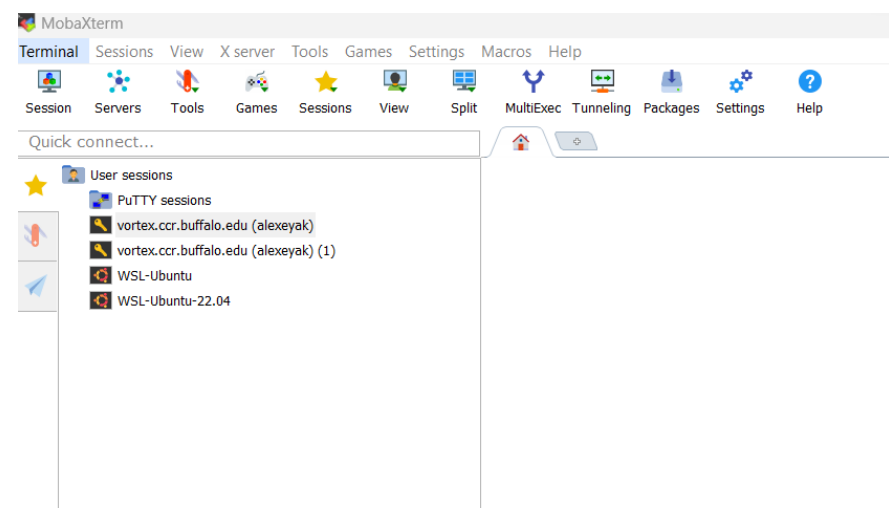


Moba Xterm

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

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)"
```

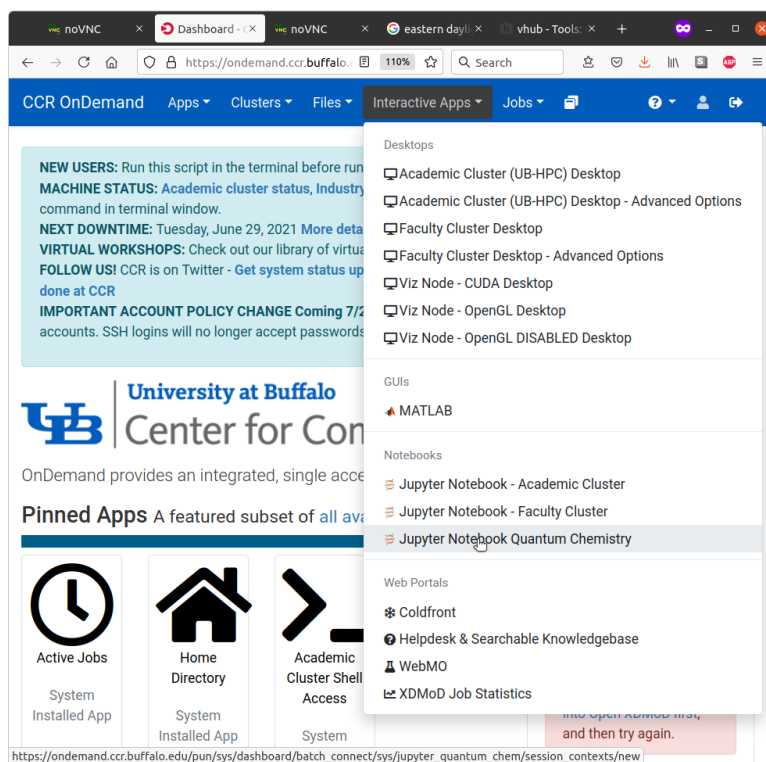
- Restart terminal or `source .bashrc`
- For terminal-based operations: Activate conda environment: `conda activate libra2`
- For Jupyter – just launch it

Projects directory: `/projects/academic/cyberwksp21` - slower, smaller, but permanent

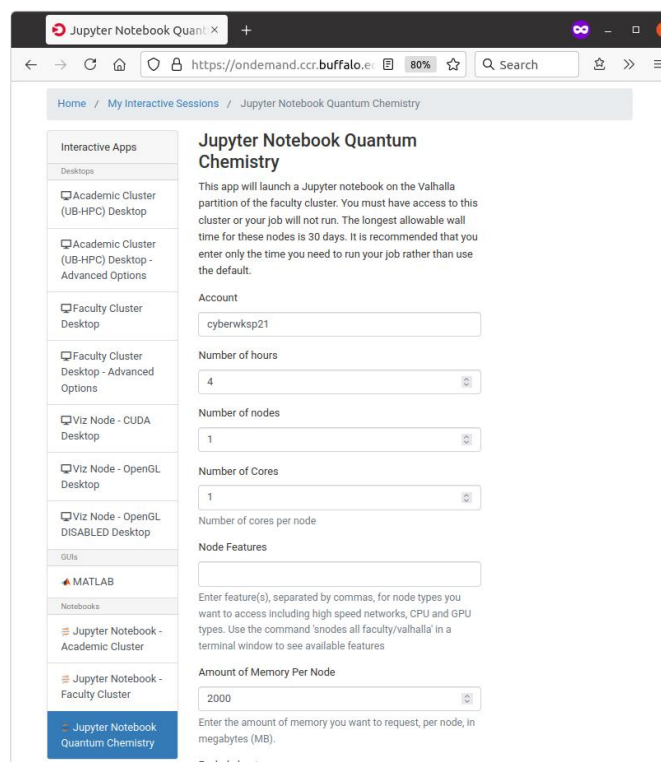
Scratch space: `/panasas/scratch/grp-cyberwksp21` - faster, larger, but temporarily (unused files are cleaned up every 1 or 2 weeks)

Using Jupyter Notebooks

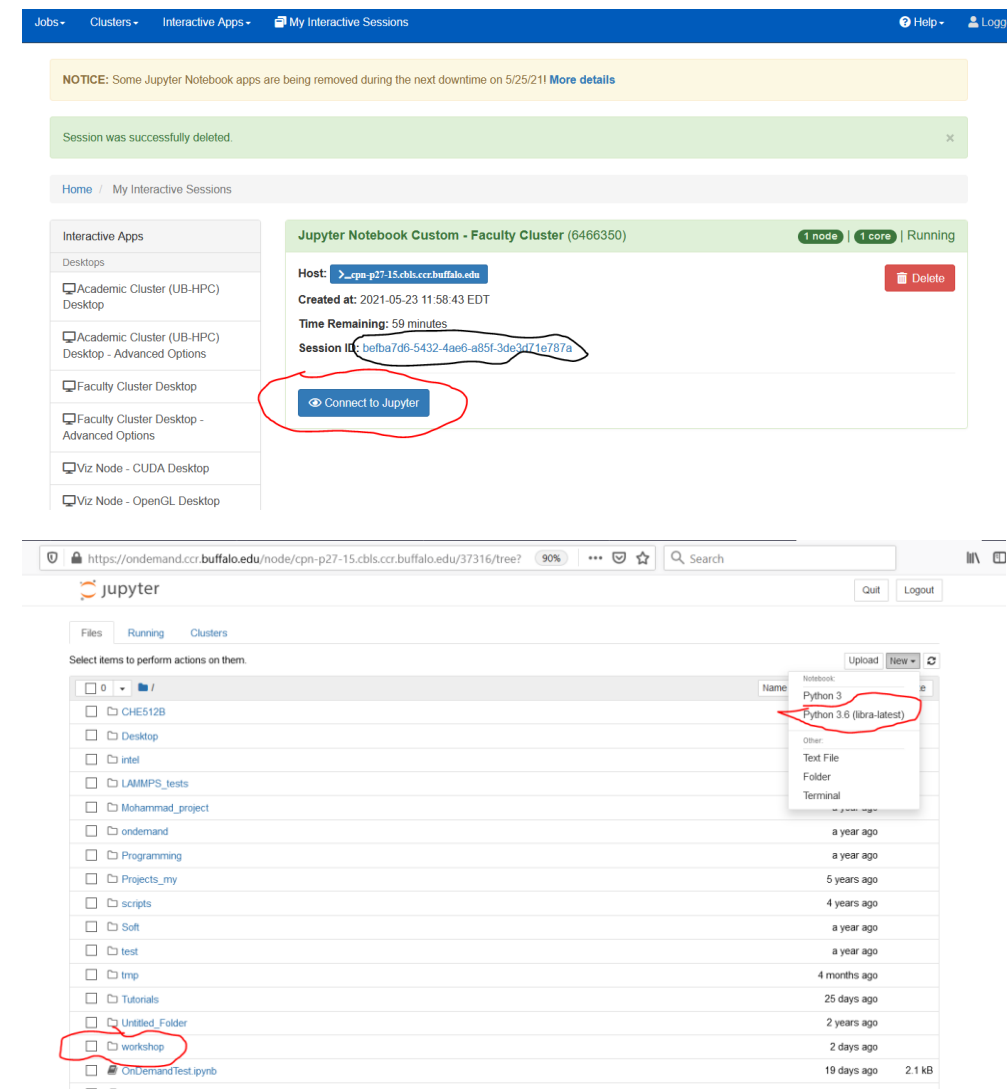
[https://compchem-cybertraining.github.io/Cyber Training Workshop 2023/ episodes/01-introduction](https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2023/episodes/01-introduction)



The screenshot shows the CCR OnDemand dashboard. The 'Interactive Apps' menu is open, displaying a list of desktops and GUIs. Under 'Desktops', options include 'Academic Cluster (UB-HPC) Desktop', 'Faculty Cluster Desktop', and 'Viz Node - CUDA Desktop'. Under 'GUIs', 'MATLAB' is listed. The 'Pinned Apps' section shows 'Jupyter Notebook - Academic Cluster', 'Jupyter Notebook - Faculty Cluster', and 'Jupyter Notebook Quantum Chemistry'.



The screenshot shows the configuration page for 'Jupyter Notebook Quantum Chemistry'. It includes fields for 'Account' (cyberwks21), 'Number of hours' (4), 'Number of nodes' (1), 'Number of Cores' (1), and 'Node Features'. The 'Amount of Memory Per Node' is set to 2000 MB.



The screenshot shows the Jupyter Notebook interface. The 'Files' tab is active, displaying a file explorer. The 'workshop' directory is highlighted. A context menu is open over the 'workshop' directory, showing options like 'Python 3', 'Python 3.6 (libra-latest)', 'Text File', 'Folder', and 'Terminal'. The 'Python 3.6 (libra-latest)' option is highlighted.