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Libra Summer School and Workshop 2024

Alexey Akimov, Sophya Garashchuk, Mohammad Shakiba, Daeho Han, Qingxin Zhang

University at Buffalo, SUNY

July 8, 2024

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Libra Summer School/Workshop

Goals and Objectives

Scientific Software Availability is essential

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PRL 95, 163001 (2005) PHYSICAL REVIEW LETTERS week ending 14 OCTOBER 2005

Trajectory Surface Hopping in the Time-Dependent Kohn-Sham Approach for Electron-Nuclear Dynamics

Colleen F. Craig, Walter R. Duncan, and Oleg V. Prezhdo*
Department of Chemistry, University of Washington, Seattle, Washington 98195-1700, USA
(Received 25 May 2005; published 10 October 2005)

Oleg Prezhdo

FOLLOW

Professor of Chemistry, and Physics and Astronomy, University of Southern California
Verified email at usc.edu - Homepage
quantum dynamics nanoscale systems solar energy

TITLE	CITED BY	YEAR
Trajectory Surface Hopping in the Time-Dependent Kohn-Sham Approach<? format?> for Electron-Nuclear Dynamics CF Craig, WR Duncan, OV Prezhdo Physical review letters 95 (16), 163001	732	2005
Theoretical Studies of Photoinduced Electron Transfer in Dye-Sensitized TiO_2 WR Duncan, OV Prezhdo Annu. Rev. Phys. Chem. 58 (1), 143-184	660	2007
The PYXAID program for non-adiabatic molecular dynamics in condensed matter systems AV Akimov, OV Prezhdo Journal of chemical theory and computation 9 (11), 4959-4972	631	2013
Decoherence-induced surface hopping HM Jaeger, S Fischer, OV Prezhdo The Journal of chemical physics 137 (22)	551	2012
Theoretical insights into photoinduced charge transfer and catalysis at oxide interfaces AV Akimov, AJ Neukirch, OV Prezhdo Chemical reviews 113 (6), 4496-4565	509	2013
Advanced capabilities of the PYXAID program: integration schemes, decoherence effects, multiexcitonic states, and field-matter interaction AV Akimov, OV Prezhdo	484	2014

JCTC Journal of Chemical Theory and Computation — Article — pubs.acs.org/JCTC

The PYXAID Program for Non-Adiabatic Molecular Dynamics in Condensed Matter Systems

Alexey V. Akimov[†,‡] and Oleg V. Prezhdo*[,†]
[†]Department of Chemistry, University of Rochester, Rochester, New York 14627, United States
[‡]Chemistry Department, Brookhaven National Laboratory, Upton, New York 11973, United States

Challenges:

- too many scripts, the connections are unclear (long training time)
- Fortran (quite "bulky"), Perl for workflow (intimidating to understand), poor modularity – difficult to add new methods
- Interfaced only with VASP
- Internal, not available to the publi
- No structured tutorials

Alexey V Akimov

FOLLOW

Associate Professor, University at Buffalo, SUNY
Verified email at buffalo.edu - Homepage
quantum and molecular dy… electronic structure theory nanotechnology and materi…

TITLE	CITED BY	YEAR
The PYXAID program for non-adiabatic molecular dynamics in condensed matter systems AV Akimov, OV Prezhdo Journal of chemical theory and computation 9 (11), 4959-4972	631	2013
Theoretical insights into photoinduced charge transfer and catalysis at oxide interfaces AV Akimov, AJ Neukirch, OV Prezhdo Chemical reviews 113 (6), 4496-4565	509	2013
Advanced capabilities of the PYXAID program: integration schemes, decoherence effects, multiexcitonic states, and field-matter interaction AV Akimov, OV Prezhdo Journal of chemical theory and computation 10 (2), 789-804	484	2014
Recent progress in surface hopping: 2011–2015 L Wang, A Akimov, OV Prezhdo The journal of physical chemistry letters 7 (11), 2100-2112	352	2016
Large-Scale Computations in Chemistry: A Bird's Eye View of a Vibrant Field A Akimov, O Prezhdo Chem. Rev.	227	2015

Changes:

- more clear workflow organization
- C++ and Python, more modular and user-friendly interface. As a result: added new methods (decoherence)
- Interfaced with QE, but not only
- Publicly available, open-source
- Dedicated tutorials

Oleg's 1-st most cited paper (excluding 2 review)

Oleg's 2-nd most cited paper (excluding 2 reviews)

My 1-st most cited paper (excluding 1 review)

Still not sufficient: Libra motivation

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- Many codes (Newton-X, SHARC, NEXMD, FIERBALL, JADE, MOLPRO, PYXAID, PYUNIXMD, …)
  - Black-box. Difficult to re-use to formulate other methods, etc.
  - Limited functionality (high focus, e.g. atomistic of special kind)

- Many methods (FSSH, DISH, A-FSSH, QTAG, QTSH, etc.)
  - Not always available
  - Not always user-friendly (e.g. my experience with PYXAID prototype)
  - Not always portable/modular, lack of best coding standards, no version control, etc.
  - Limited consistency of different codes
  - Possible redundancies even in the same code

- Libra's approach
  - Versatility: encompass a comprehensive set of available methodologies
  - Community-centric: be the platform for various methods developed by the community
  - Modularity: easy-to-use methodology building blocks, methodology development
  - User-friendliness & Open-source: easy experience, without limitations

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

Libra motivation

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The key “software” papers

☐	Libra: an open-source “methodology discovery” library for quantum and classical dynamics simulations AV Akimov Journal of computational chemistry 37 (17), 1626-1649	80	2016
☐	Libra: A modular software library for quantum nonadiabatic dynamics M Shakiba, B Smith, W Li, M Dutra, A Jain, X Sun, S Garashchuk, ... Software Impacts 14, 100445	12	2022

- Many changes compared to Pyxaid – a lot of correctness issues fixed, more reliable approach
- Nearly all the projects in my lab use it
- There is a growing number of users who use it – that’s another reason to host this event

- Adopt the best practices
  - Modularity (e.g. PySCF, Psi4NumPy, PyQuante, HORTON)
  - Language standards (Python, C++ vs. Fortran? Hybrid programming)
  - Testing & Documentations (pytest, unittest, Doxygen/Sphinx)
  - User/developer training (Workshops, Summer/Winter schools)
- Focus on the community
  - Every group has expertise in their field – rely on that
  - Community contributions – PR on GitHub
  - Use version control and collaborative workflows via GitHub, Issues
  - Frequent communication and close collaboration e.g. via Slack

Some papers that use Libra

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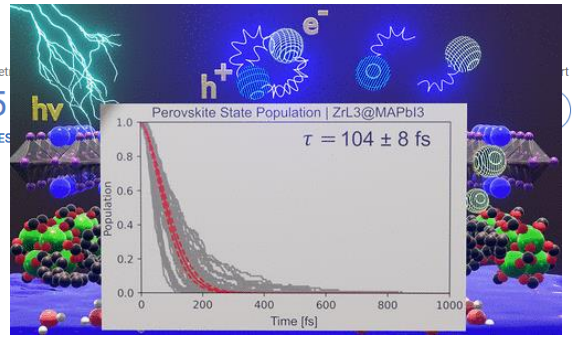
RETURN TO ISSUE | < PREV | LETTER | NEXT >

Charge Carrier Dynamics at the Interface of 2D Metal–Organic Frameworks and Hybrid Perovskites for Solar Energy Harvesting

Robert Stanton and Dhara J. Trivedi*

Cite this: *Nano Lett.* 2023, 23, 24, 11932–11939
Publication Date: December 15, 2023
https://doi-org.gate.lib.buffalo.edu/10.1021/acs.nanolett.3c04054

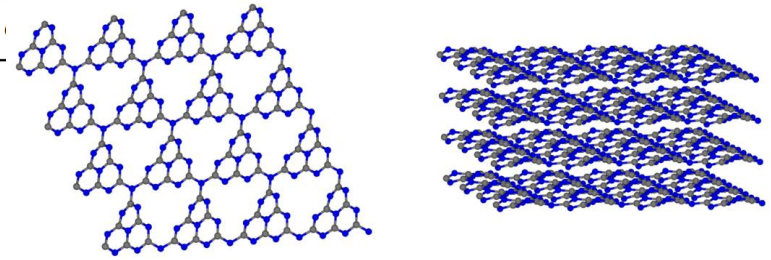
Article Views 675 | Altmet 5
LEARN ABOUT THES



Ab initio quantum dynamics of charge carriers in graphitic carbon nitride nanosheets

Cite as: J. Chem. Phys. **153**, 054701 (2020); https://doi.org/10.1063/5.0010628
Submitted: 13 April 2020 • Accepted: 11 June 2020 • Published Online: 03 August 2020

Sraddha Agrawal, Wei Lin,



Angewandte International Edition Chemie | GDCh | A Journal of the German Chemical Society

Research Article | Full Access

Insight into the Molecular Mechanism for Enhanced Longevity of Supramolecular Vesicular Photocatalysts

Dr. Yannan Liu, Dr. Fulu Zheng, Haojie Dai, Chuanshuang Chen, Yajing Chen, Dr. Haolin Wu, Prof. Chunyang Yu, Prof. Yiyong Mai, Prof. Thomas Frauenheim, Prof. Yongfeng Zhou

First published: 13 April 2023 | https://doi-org.gate.lib.buffalo.edu/10.1002/anie.202302126 |
Citations: 2

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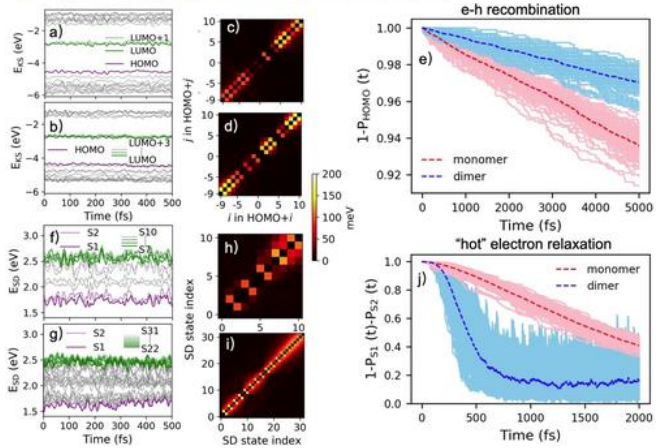
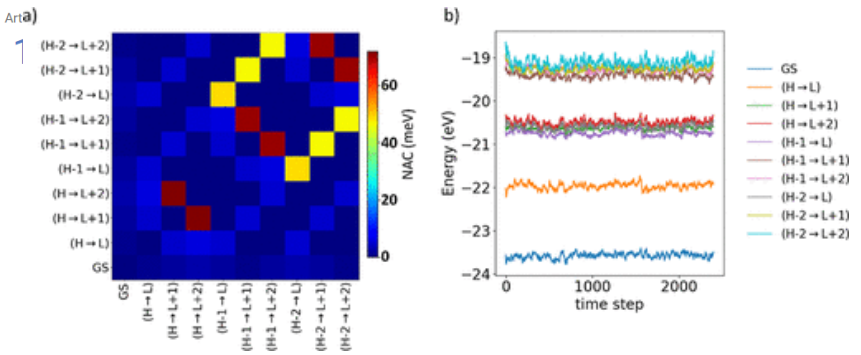


RETURN TO ISSUE | < PREV | A: NEW TOOLS AND MET... | NEXT >

Convergence of Time-Derivative Nonadiabatic Couplings in Plane-Wave DFT Calculations

Alva D. Dillon and Rebecca L. M. Gieseking*

Cite this: *J. Phys. Chem. A* 2023, 127, 45, 9612–9620
Publication Date: November 4, 2023
https://doi-org.gate.lib.buffalo.edu/10.1021/acs.jpca.3c04858



+ many works in my group
+ upcoming works

Objectives of this Workshop/Summer School

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"Elements: Libra: The Modular Software for Nonadiabatic and Quantum Dynamics"

- Develop new functionality in the Libra code
- Train users/developers & facilitate the adoption by the community (this workshop)
- Visitations for the collaborators

Objectives:

- Learn what is available, the best practices, known pitfalls
- Learn to conduct atomistic and model calculations (theory and practice)
- Learn internals, so that you could potentially contribute

Overarching goal: become the code's user and/or developer

Why to contribute?

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- Make your methods broadly available (mutually advertise)
- Be listed on the developers/contributors lists, get credentials, get citations

- Make your methods compatible with other methods, enable easier interfacing – this facilitates new methods developments
- Take advantage of other methods/functions/data types available in the same code – learn once then swim
- Take advantage of improvements of other parts of the code
- Mutually ensure the best standards and facilitate bug discovery/testing

How to contribute?

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Received: 18 April 2020 | Revised: 19 May 2020 | Accepted: 8 June 2020
DOI: 10.1002/qua.26373

Check for updates

SOFTWARE NEWS & UPDATES

International Journal of Quantum Chemistry WILEY

Hierarchical equations of motion in the Libra software package

Story Temen[1] | Amber Jain[2] | Alexey V. Akimov[1]

[1]Department of Chemistry, University at Buffalo, The State University of New York, Buffalo, New York, USA

Abstract

We report the implementation of a hierarchical equations of motion (HEOM) module

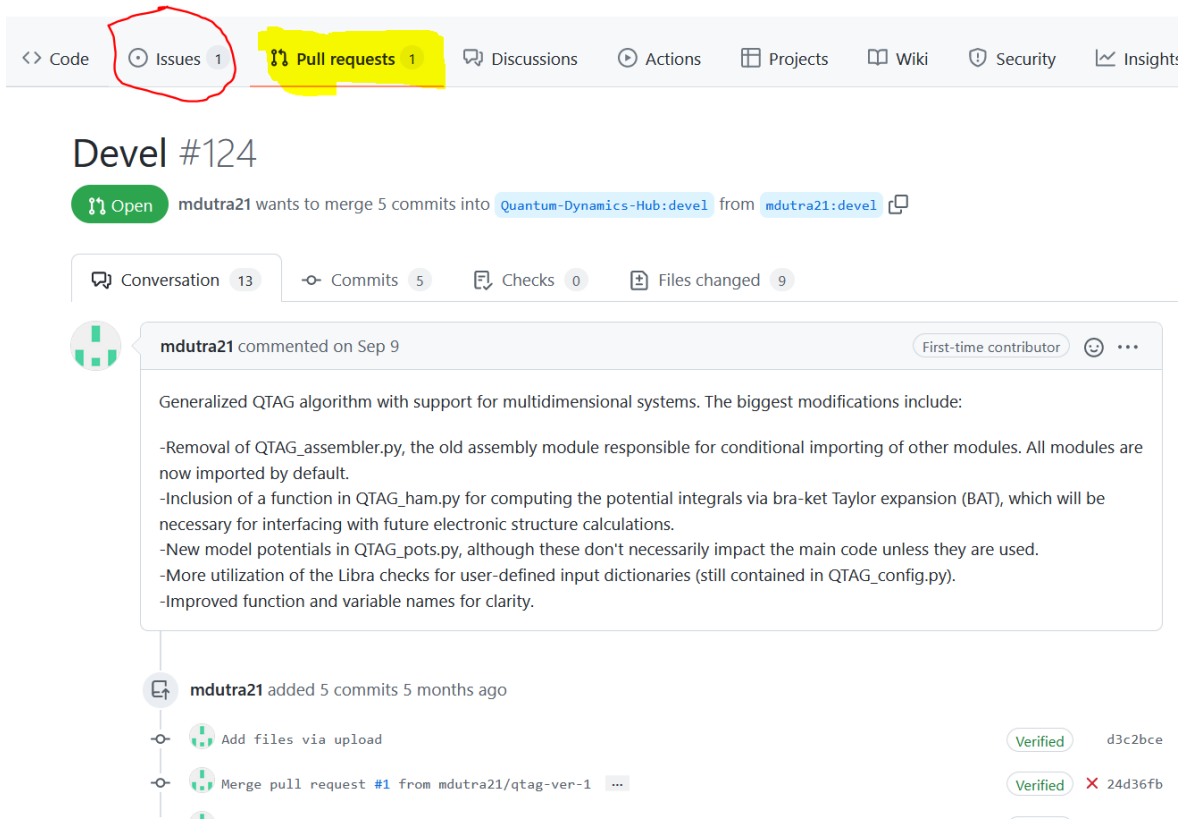
https://github.com/amber-jain-group-iitb/heom_amber

Before:

- hard-coded inputs (recompile for all parameters)
- Fortran into executable

After:

- General-purpose code, any inputs
- Python/C++, integrate with the plotting scripts, etc.



- create a pull-request
- open an issue
- start a discussion (haven't tried yet)

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Libra Summer School/Workshop

Logistics & Agenda

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Getting to Know Each Other

Instructors and Co-Instructors

University at Buffalo
The State University of New York

Alexey Akimov
TSH, SOFT, HEOM

Sophya Garashchuk
QTAG

Mohammad Shakiba
Atomistic NBRA-NA-MD, ML, CP2K

Daeho Han
XF

Qingxin Zhang
Atomistic NBRA-NA-MD, CP2K

Please Introduce Yourself

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

The Plan & Resources

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All the details are here:

https://compchem-cybertraining.github.io/Libra_Summer_School_2024/

Libra Workshop and Summer School on Excited States and Nonadiabatic Dynamics 2024

Join Slack:

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

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

VPN and Accounts:

- setup now, instruction by Ms. Dori Sajdak
- 2-factor authentication
- submit a ticket: https://ubccr.freshdesk.com/support/home

Resources: Past Events

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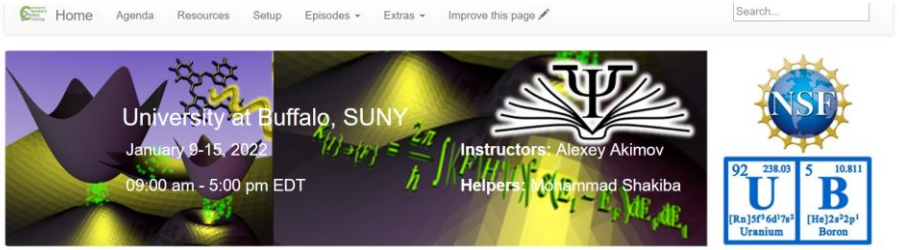
This is the second event on Libra:

The first one – Winter 2022:

https://compchem-cybertraining.github.io/Libra_Winter_School_2022/



Libra Winter School on Excited States and Nonadiabatic Dynamics in Materials 2022

Comutational Chemistry CyberTraining https://github.com/compchem-cybertraining

Learning Libra: The dedicated set of tutorials: https://github.com/compchem-cybertraining/Tutorials_Libra

Learning Libra AND theory AND other packages: CyberTraining workshops

- 2023: https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2023/
- https://github.com/compchem-cybertraining/Cyber_Training_Workshop2023_course_projects

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

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

Excited States and Nonadiabatic Dynamics CyberTraining Workshop 2023

Event Plan

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https://compchem-cybertraining.github.io/Libra_Summer_School_2024/schedule.html

1. Monday: Introduction, Libra overview, Presentations
2. Tuesday: Model Hamiltonian setups, Quantum, TSH/Ehrenfest, and HEOM calculations for model problems.
3. Wednesday: QTAG, VISTA, Exact factorization (XF)
4. Thursday: TSH calculations for atomistic systems
5. Friday: Machine learning for atomistic systems

Notes:

1. The focus is to apply these skills to your own systems, not just to follow the tutorials
2. Some tasks are interconnected – you will use the results of your calculations in later stages
3. Plenty time for discussion and collaboration on every day: Not just the tutorials

Daily Schedule

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Daily

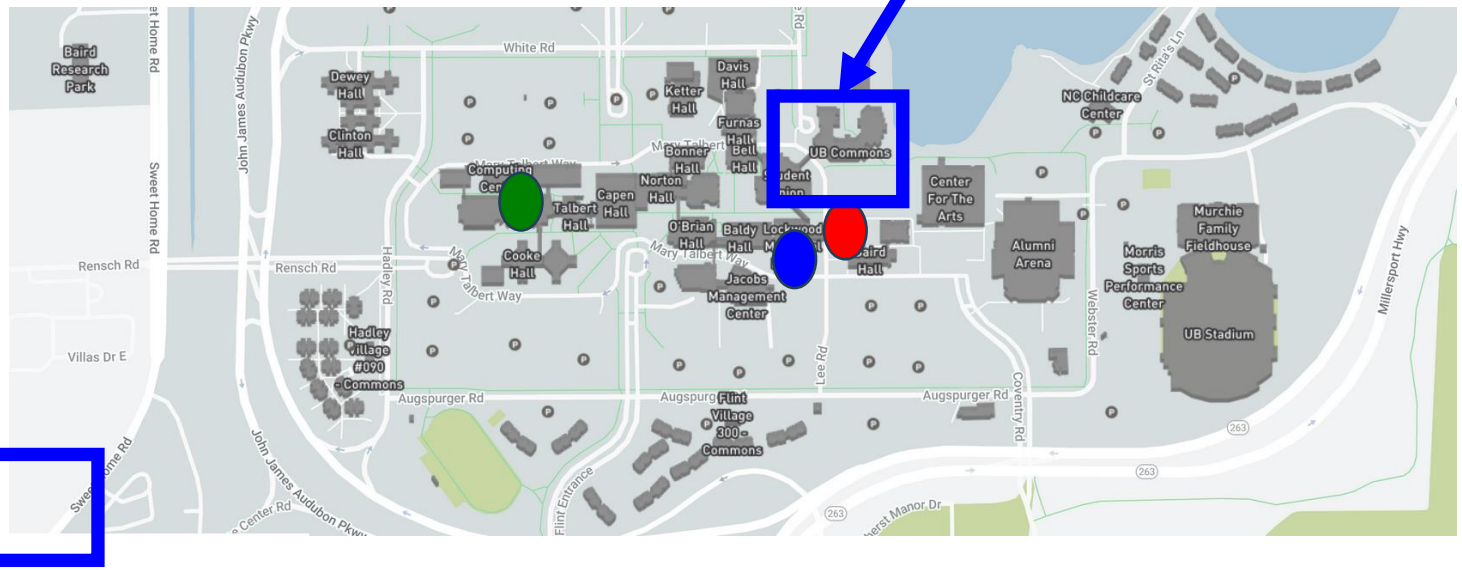
- Breakfast = hotel
- 9:00 am – 12:00 pm: Morning session (Recording)
- 12:00 – 1:30 pm Working lunch/rest – on your own at “Commons”, rest, discuss, collaborate
- 1:30 pm – 5:00 pm: Afternoon session (Recording)
- After 5:00 pm: collaborations/on your own, dinner on your own

Location

- Classes are @: July 8, 9 – Clemens 120
- July 10, 11 – NSC 220
- July 12 – Baldy Hall 200G

Eat here

Your hotel plaza



Campus Map: https://www.buffalo.edu/home/visiting-ub/map.html

Post-workshop – Reimbursement & Accounts

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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/car expenses via Slack (DM)

- 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

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

- You UB CCR accounts will be valid until end of August – feel free to use them as needed (but don't forget to acknowledge it if it results in a publication).

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Getting Started on UB CCR

Accessing UB Computing Resources

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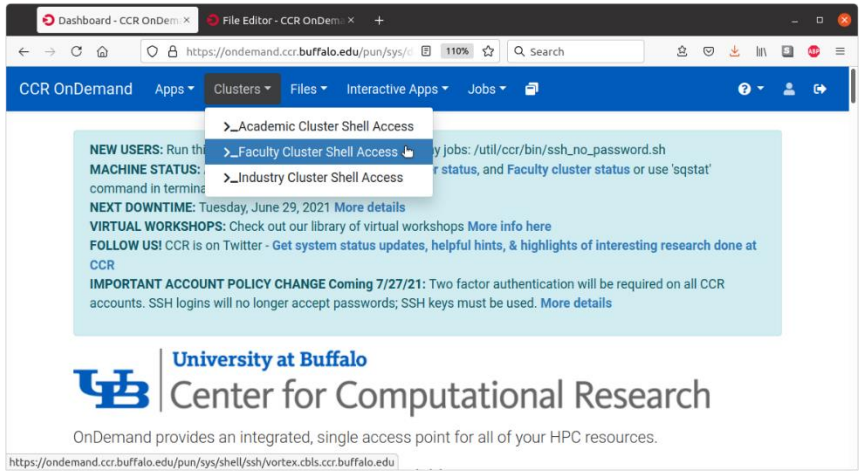
Before the Workshop

https://compchem-cybertraining.github.io/Libra_Summer_School_2024/setup.html

OnDemand

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

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

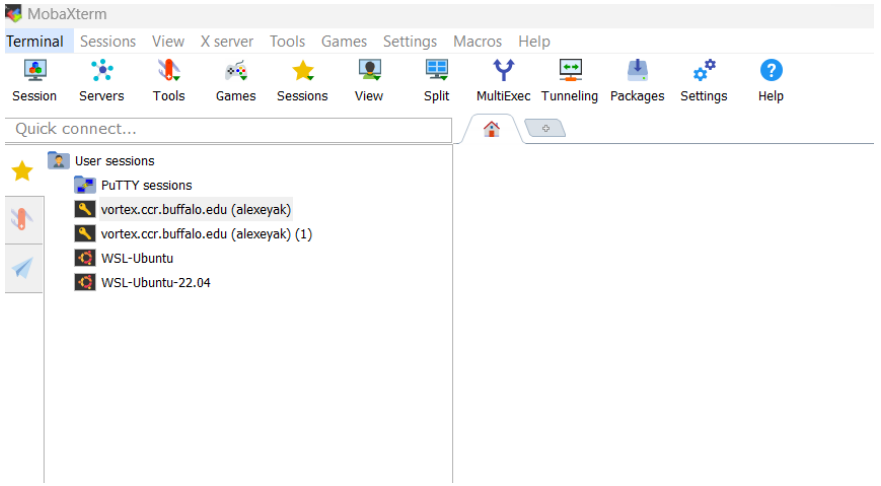


Moba Xterm

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)

https://akimovlab.github.io/soft_and_tuts/3.4-libra.html

```
# .bashrc
# User specific aliases and functions
# Source global definitions
if [ -f /etc/bashrc ]; then
        . /etc/bashrc
fi
module use /projects/academic/cyberwksp21/MODULES module load libra/devel export
PYTHONPATH=/projects/academic/cyberwksp21/SOFTWARE_NEW_ENV/libra/devel/_build/src:$PYTHONPATH export
LD_LIBRARY_PATH=/projects/academic/cyberwksp21/SOFTWARE_NEW_ENV/libra/devel/_build/src:$LD_LIBRARY_PATH
```

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

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

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

Using Jupyter Notebooks

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https://akimovlab.github.io/soft_and_tuts/3.4-libra.html