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Excited States and Nonadiabatic Dynamics
CyberTraining School/Workshop 2023

Alexey Akimov

University at Buffalo, SUNY

June 11, 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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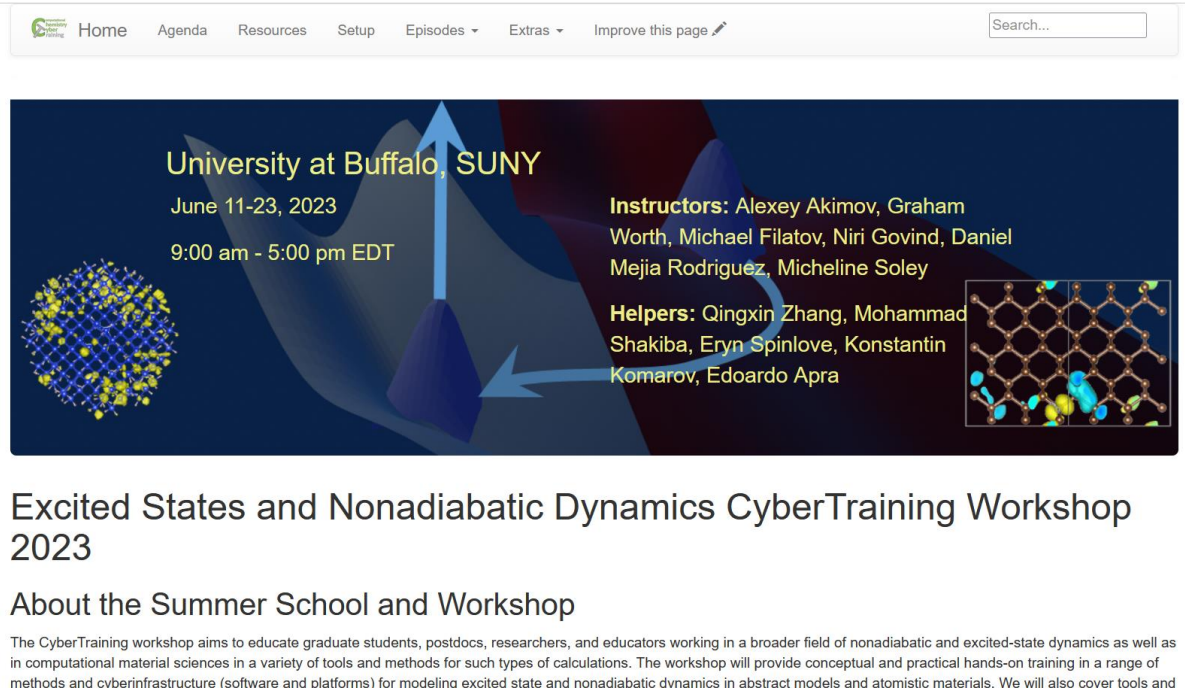
All the details are here:

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 and Demo/Hands on)(90 min) **Noon - 1:30 pm** Lunch break **Afternoon, 1:30 pm - 5:00 pm** • Theory of adiabatic and nonadiabatic dynamics. Lecture (60 min) • TSH and Ehrenfest dynamics with model Hamiltonians in Libra. Hands on (90 min) • HEOM and QTAG in Libra. (60 min)	Alexey Akimov, Qingxin Zhang, Mohammad Shakiba
June 13, 2023 (Day 3), Tuesday	**Morning, 9 am - noon** • Machine learning capabilities of Libra: Lecture, Demo, and Hands on (60 min) • DVR in Libra. Lecture, Demo, and Hands on (90 min) • TBD (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

Topics and Instructors

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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

Topics and Instructors

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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)

Topics and Instructors

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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://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

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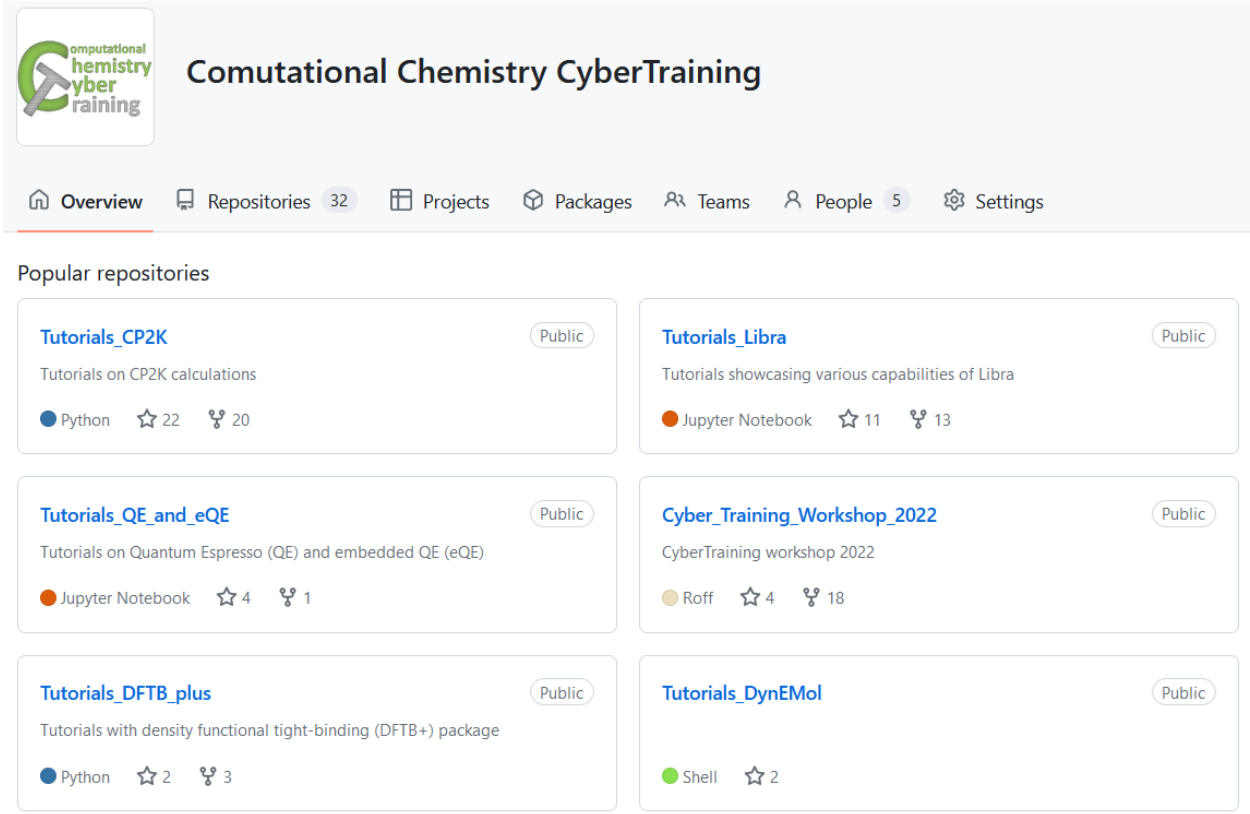
Codes: https://github.com/Quantum-Dynamics-Hub
Training: https://github.com/compchem-cybertraining

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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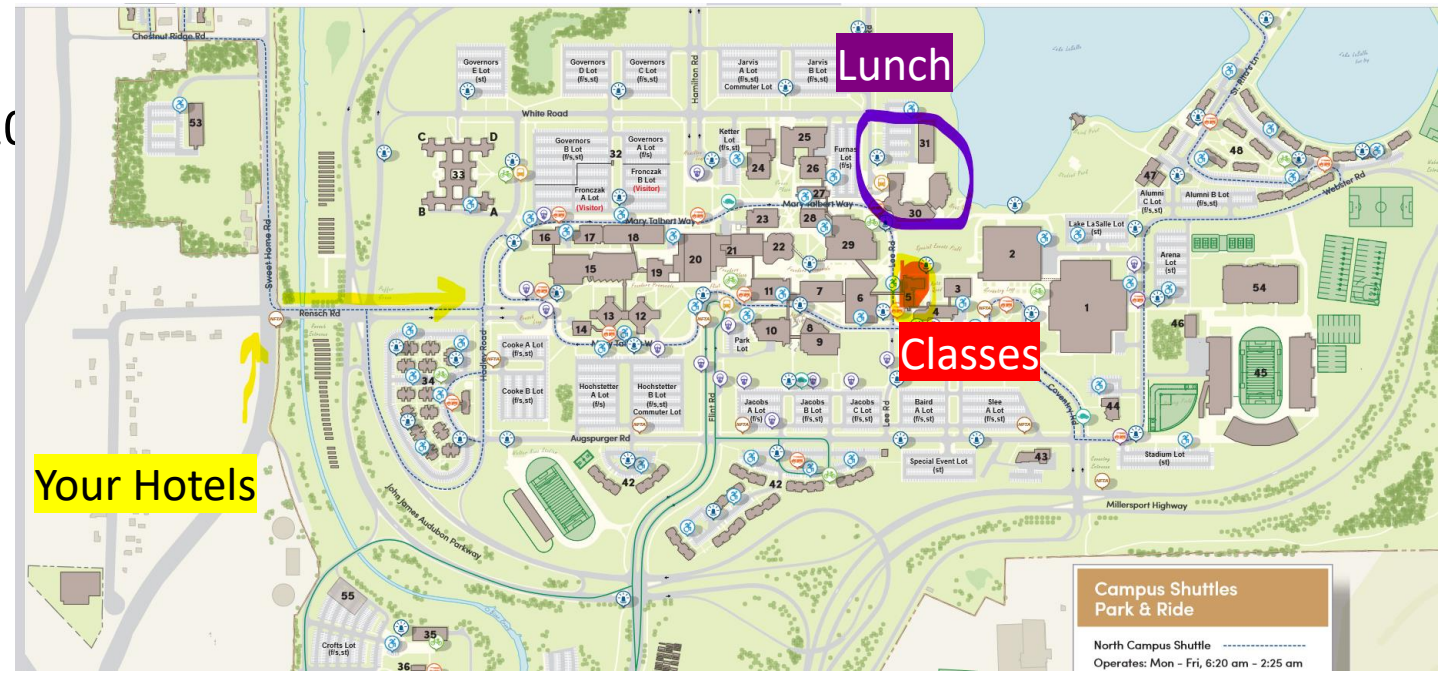
Daily

- 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

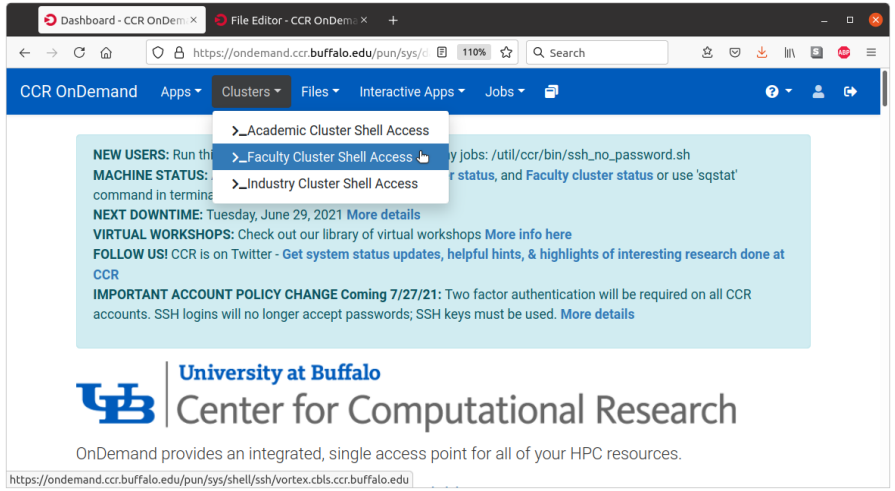
https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2023/setup.html

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/

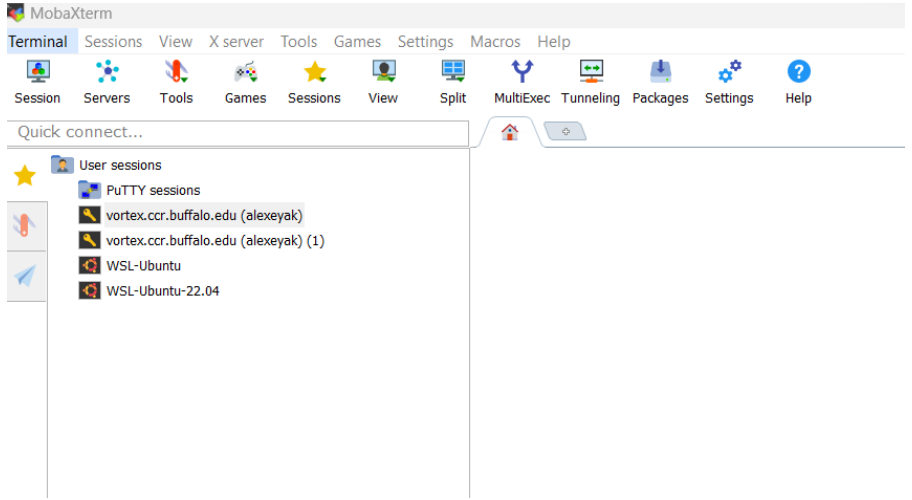


Moba Xterm

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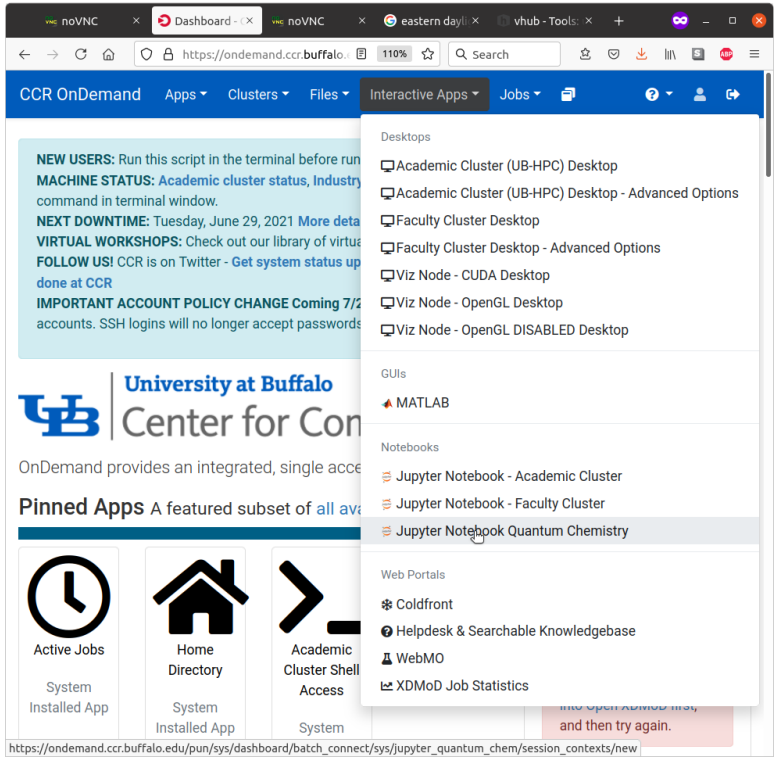
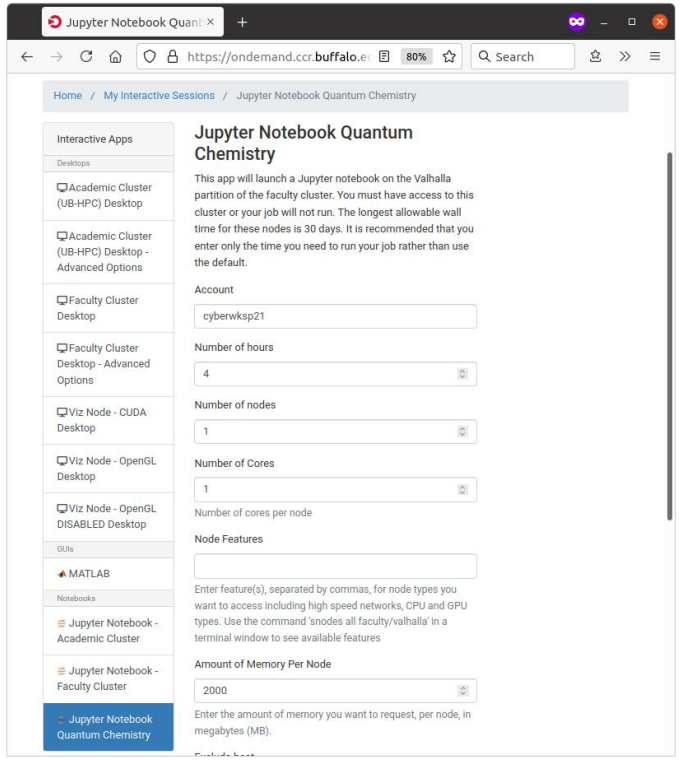
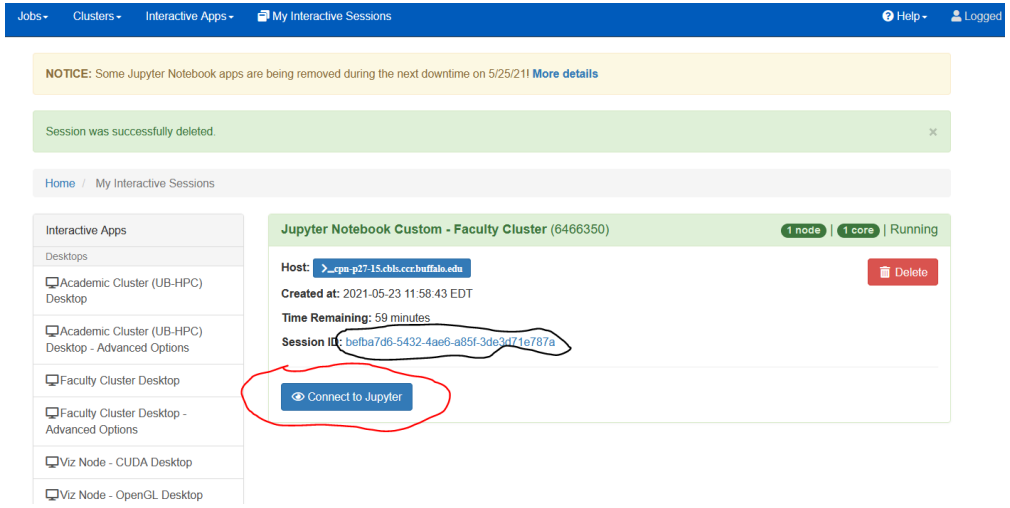
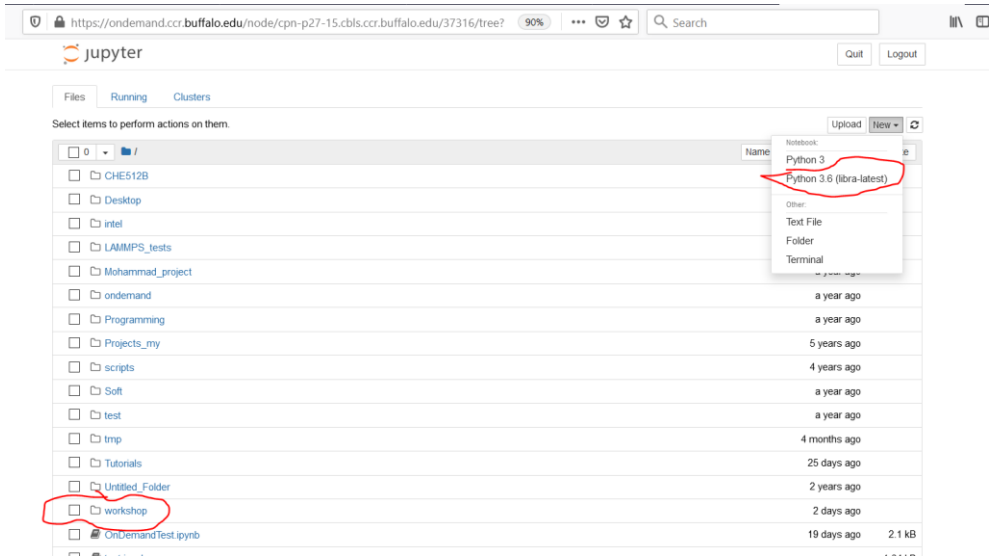
https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2023/_episodes/01-introduction









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GitHub & Git

Overview

Git and GitHub Workflow

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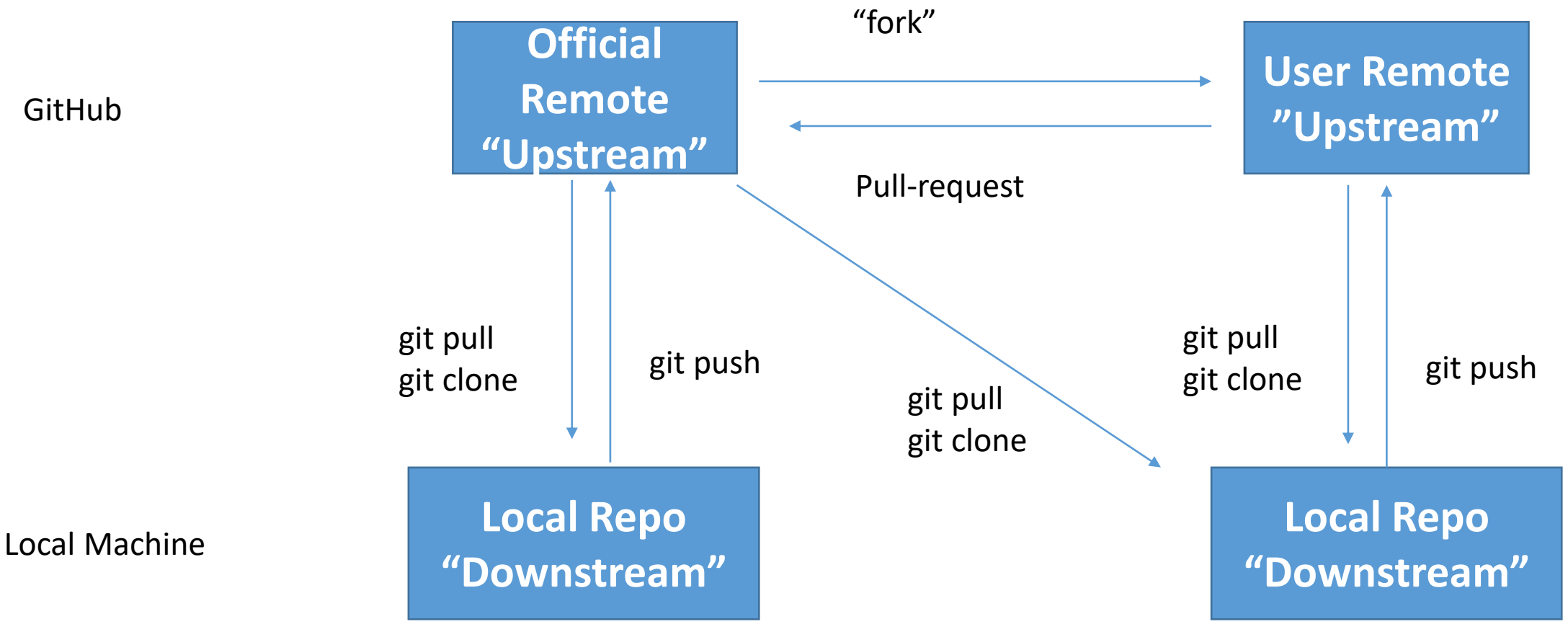

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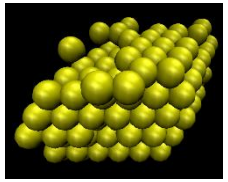
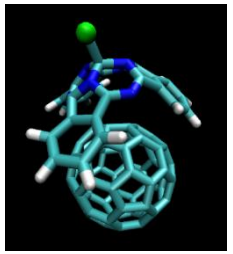
Libra overview

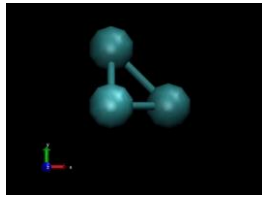
Libra History

Classical MD





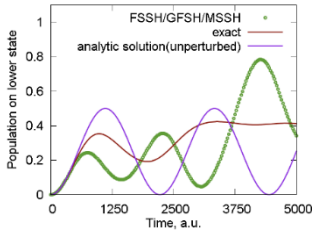
Rigid body MD

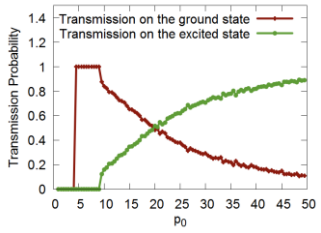


- Simplectic integrators for classical DOFs
- Thermostats
- Barostats
- Force fields
- ANN
- Chemical object representation

Akimov, Prezhdo, *JCTC,* **2013**, 9, 4959.
Akimov, Prezhdo, *JCTC*, **2014**, 10, 789

Ehrenfest & TSH

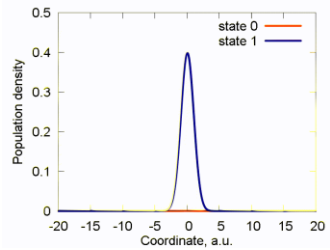




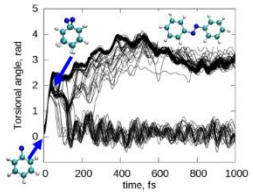
- Simplectic integrators for TDSE
- TSH, Ehrenfest, stand-alone scripts
- Decoherence methods
- Model problems
- Added HF and EHT to LCCCS
- Interface with VASP, then QE

Akimov *JCC,* **2016**, 37, 1626

DVR



Back-reaction

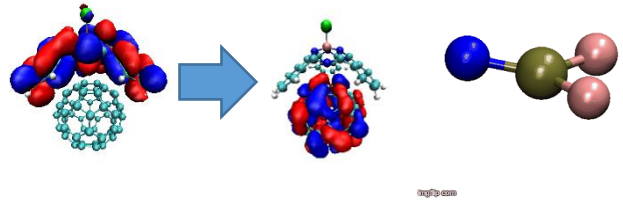


- Modularization and revision
- DVR methods
- Semiempirical Hamiltonians
- Molecular integrals
- Decoherence methods, TSH

Libra-X (with Drs. Ryoji Asahi, Kosuke Sato, Ekadashi Pradhan)

Sato, Pradhan, Asahi, Akimov *PCCP* **2018,** 20, 25275
Pradhan, Sato, Akimov *J. Phys.: Condens. Matter*, **2018**, 30, 484002

- Interfaces with GAMESS, QE
- Added back-reaction for QE
- More modularization



Pyxaid2 (with Prof. Wei Li)

Li, Zhou, Prezhdo, Akimov *ACS Energy Lett*, **2018**, 3, 2159

- SOC, multiple k-points, etc.

2007-2011 (LCCCS)

2011-2015 (Pyxaid)

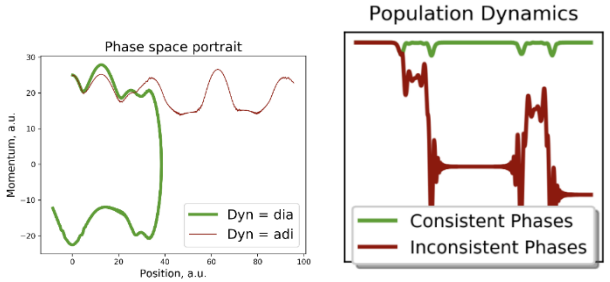
2015/2016 (Libra)

2018 (Pyxaid2, Libra-X)

Libra History

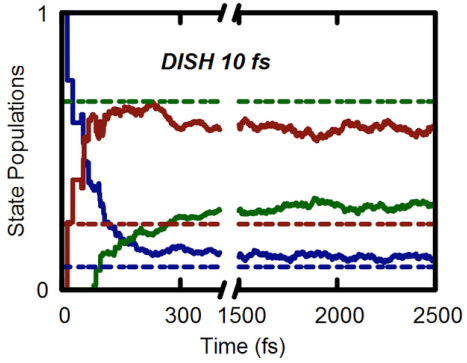
Phase correction for NACs

Akimov *JPCL* **2018** 9, 6096-6102



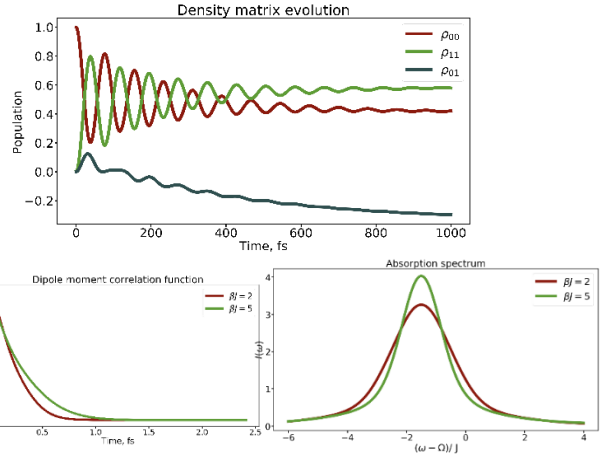
Bastida's Boltzmann-corrected Ehrenfest, mSDM

Smith; Akimov *JCP* **2019**, 151, 124107



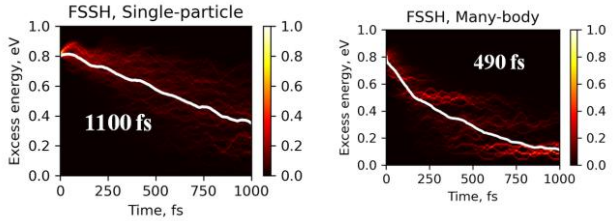
HEOM

Temen, Jain, Akimov *Int. J. Quant. Chem.*, **2020**, 120, e26373



Many-body NA-MD

Smith, B.; Shakiba, M.; AVA *JCTC* **2021**, 17, 678
Smith, B.; Shakiba, M.; AVA *JPCL* **2021**, 12, 2444

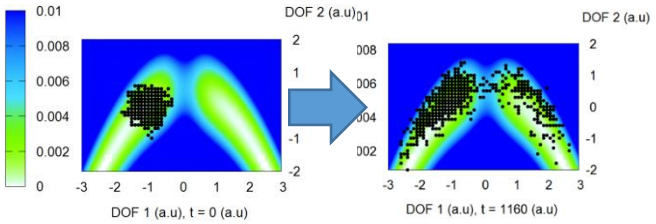


Revised DISH, new workflows

Akimov *JCP* **2021**, 155, 134106

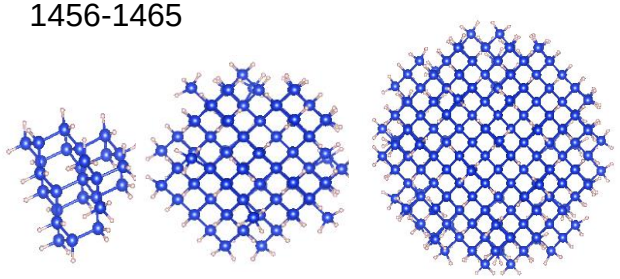
Entangled trajectories

Smith, Akimov *JCP* **2018**, 148, 144106



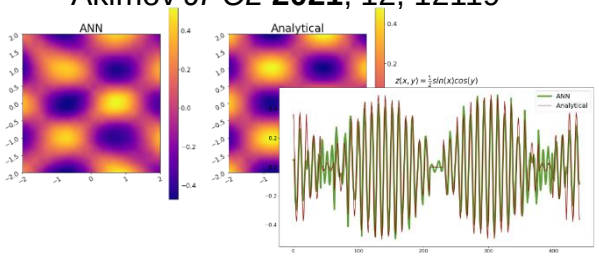
Belyaev-Lebedev LZ method

Smith, B.; Akimov, A. V *JPCL* **2020**, 11, 1456-1465



Machine Learning revised. TD-ML approach

Akimov *JPCL* **2021**, 12, 12119



2018 **2019** **2020** **2021**

Libra Philosophy/Vision

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- **modular**

  Maximize and simplify the re-use, OOP

- **versatile**

  linear algebra, integrals,
  quantum and classical mechanics/dynamics,
  nonadiabatic methods, surface hopping,
  IO utilities, model preparation and analysis

- **"methodology discovery"**
  (prototyping)

  - Use with model problems and atomistic simulations
  - Python – for convenience, C++ - for efficiency

- **practical**

  Fully-functional tool that can be applied to real (atomistic) systems to study materials

- **user-friendly & documented**

  The code is convenient to users and they have plenty resources – examples and documentation

- **community tool**

  - A platform to adopt the past and latest developments
  - The developers can understand and contribute to the code

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 Motivation

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- 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

Community Tool: Code Contributions/Integration

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Amber Jain – Hierarchical Equations of Motion (HEOM)
https://github.com/amber-jain-group-iitb/heom_amber
src/dyn/heom

Xiang Sun – (Non)-equilibrium Fermi Golden Rule (FGR)
https://github.com/tsiangsun/FGR
src/fgr

Nandini Ananth – Initial value representation (IVR)
https://github.com/AnanthGroup/SC-IVR-Code-Package
src/ivr

Sophya Garaschchuk – quantum trajectory guided Gaussians (QTAG)
src/libra_py/dynamics/qtag

Craig Martens – quantum trajectory surface hopping (QTSH)
in progress

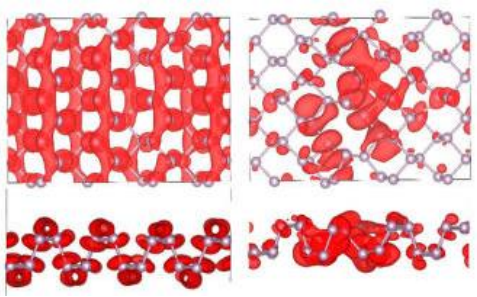
… and more

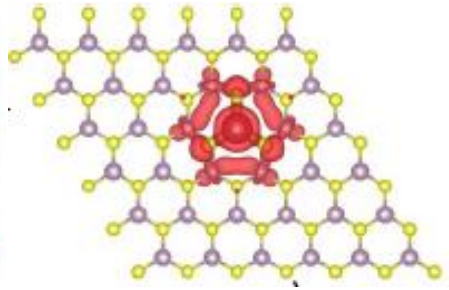
Practical: Libra in Materials Research

University at Buffalo
The State University of New York

2D systems

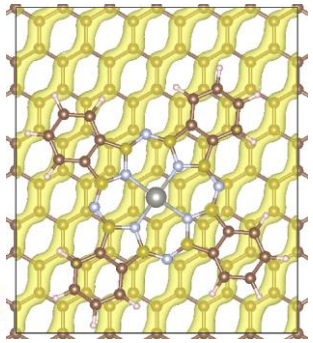
Long el al. *JPCL* **2016**, *7*, 653.

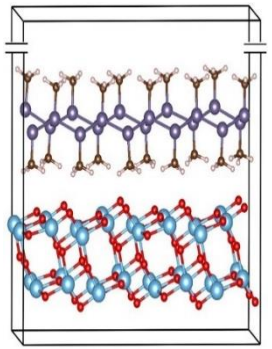




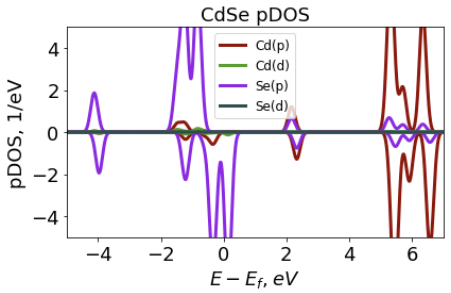
2D heterojunctions

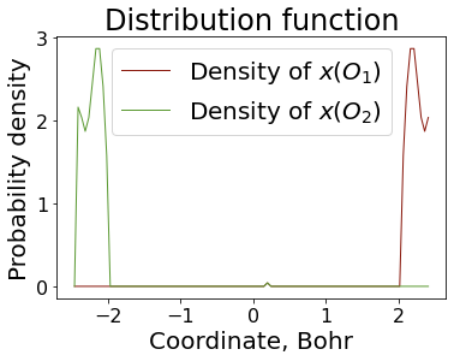
Nijamudheen, A.; AVA *JPCC*, 2017, *121,* 6520

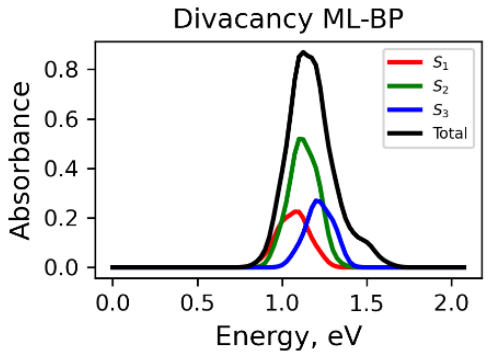




Auxiliary Analysis Tools

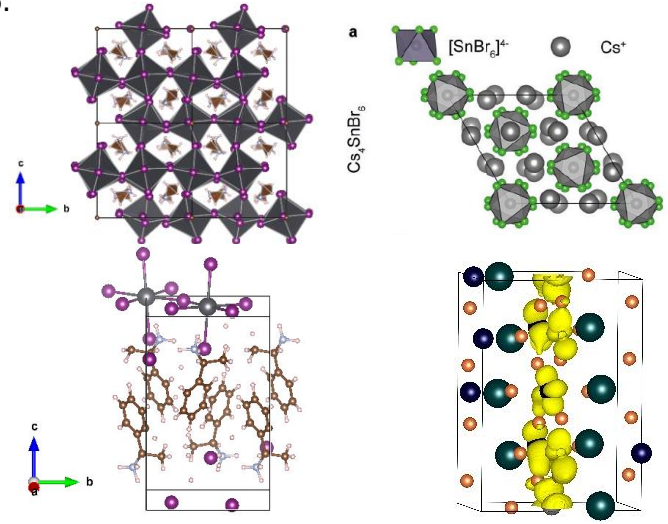






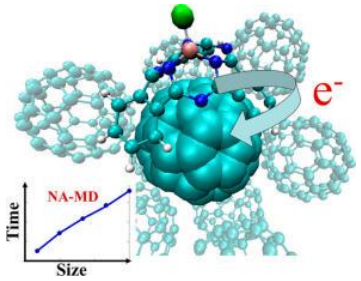
Perovskites

Nijamudheen, A.; AVA *JPCL* **2018**, *9*, 248



Organic heterojunctions

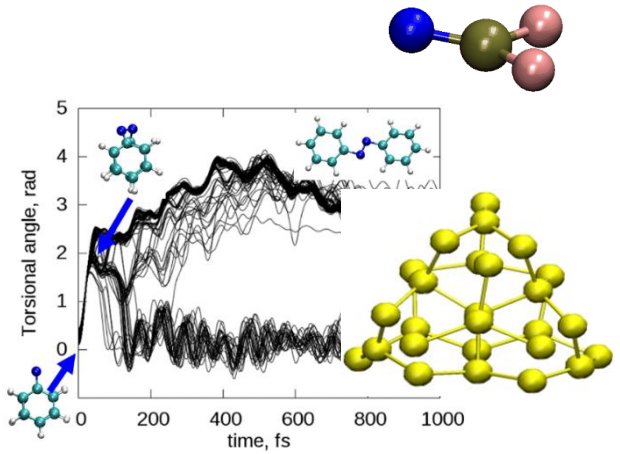
Sato et al. *PCCP,* **2018**, 20, 25275.



Quantum Dots & Molecules

Lin, Y.; AVA *JPCA.* **2016**, 120, 9028

Pradhan et al. *JPCM,* **2018**, 30, 484002



C++/Python Interoperability

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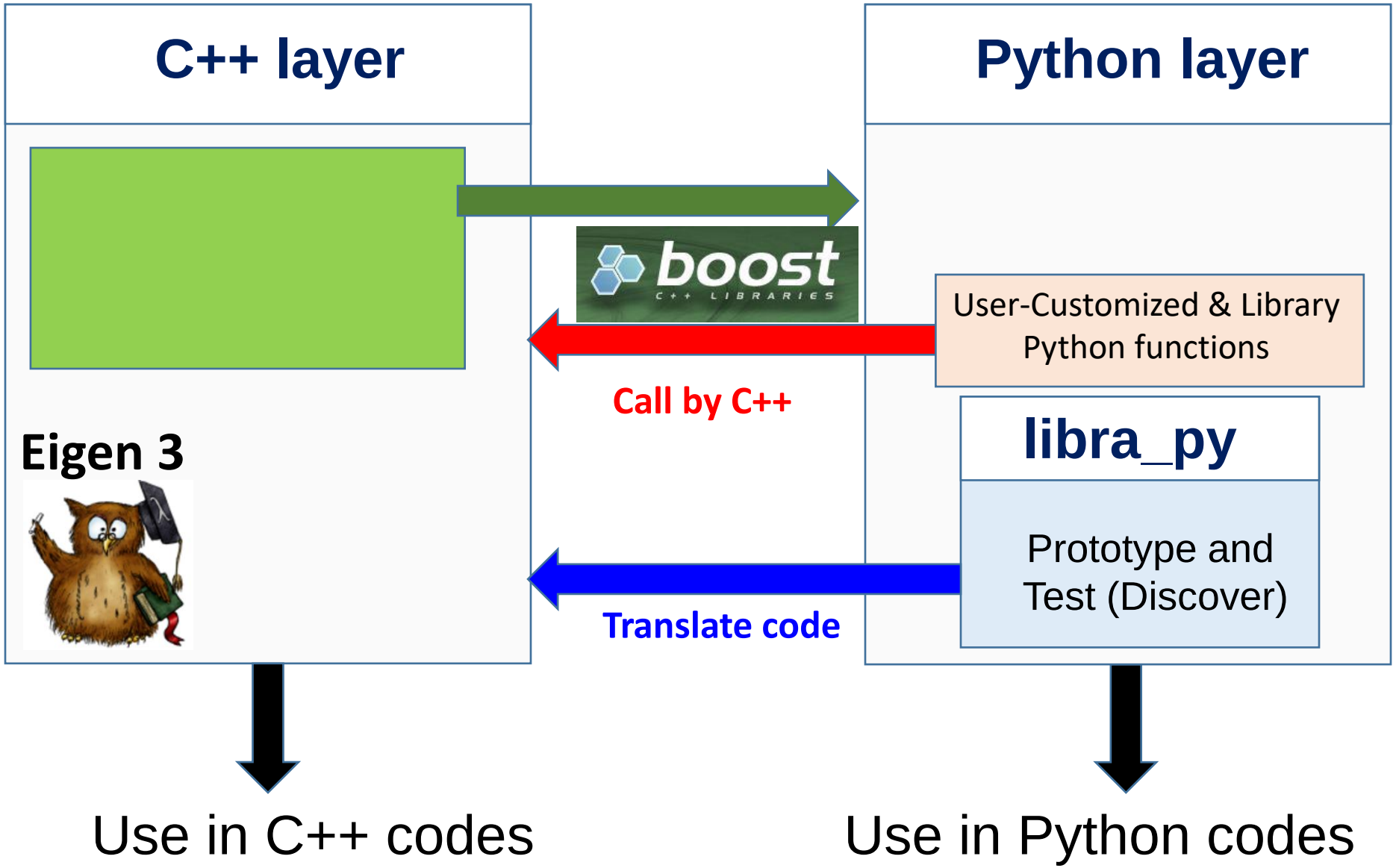

Modularity: API Diversity

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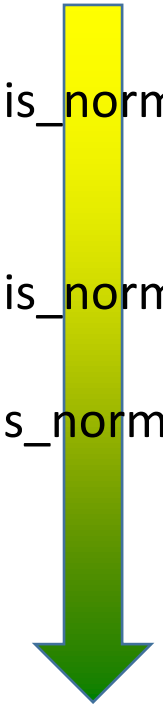
- The goal is to suite the needs of the **users of various levels**
- Find a balance between **simplicity** and **flexibility**

Developer/Efficiency



```
double gaussian_overlap( AO* AOa, AO* AOb,int is_normalize, int is_derivs,  VECTOR& dIdA, VECTOR& dIdB,
vector<double*>& auxd,int n_aux);

double gaussian_overlap( AO* AOa, AO* AOb,int is_normalize, int is_derivs, VECTOR& dIdA, VECTOR& dIdB );

double gaussian_overlap(AO* AOa, AO* AOb,int is_normalize);

double gaussian_overlap(AO* AOa, AO* AOb);
```

User/Convenience

Example

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Computing kinetic energy between Gaussians

```
g1 = PrimitiveG()
g2 = PrimitiveG()
g1.init(n1,m1,k1, a1, VECTOR(x1, y1, z1))
g2.init(n2,m2,k2, a2, VECTOR(x2, y2, z1))

kin = kinetic_integral(g1,g2)
```

Benchmarked against PyQuante

```
p1 = PyQuante.PGBF.PGBF(a1,(R1.x,R1.y,R1.z),(n1,m1,k1))
p2 = PyQuante.PGBF.PGBF(a2,(R2.x,R2.y,R2.z),(n2,m2,k2))

val_ref = p1.kinetic(p2)
```

Passing Python functions

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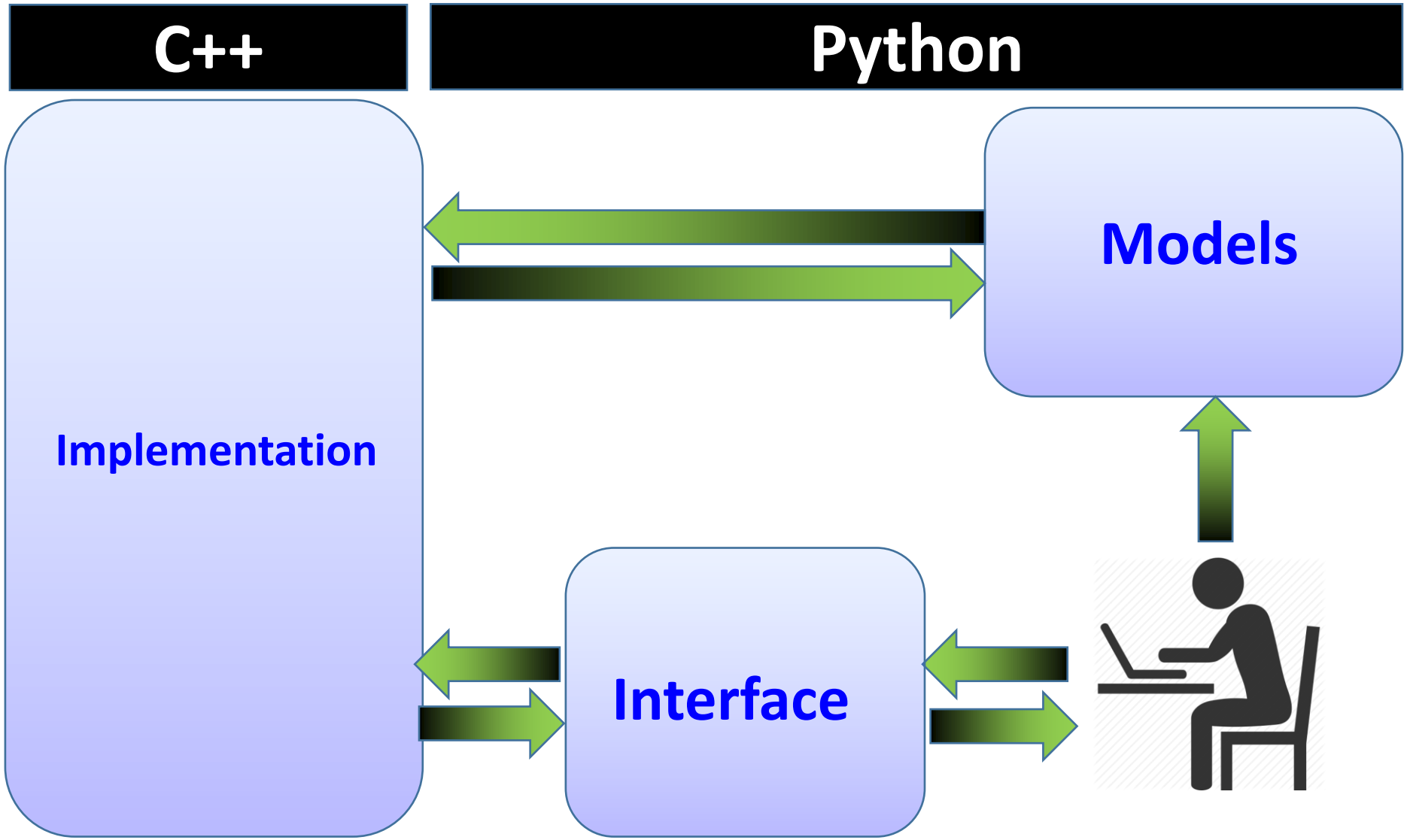

How it works with Sampling

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```
vector<MATRIX> metropolis_gau
(Random& rnd, bp::object target_distribution,
MATRIX& dof, bp::object distribution_params,
int sample_size, int start_sampling, double gau_var){
```

Metropolis Algorithm

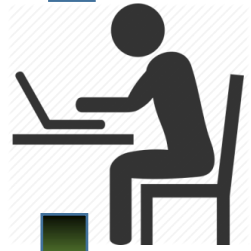
```
double p_old =
bp::extract<double>( target_distribution(s_old,
distribution_params) );

...
}
```

C++

```
def test():
  q  = MATRIX(ndof, 1)
  output = metropolis_gau( piab, q, params, ...)
```

User calls the sampling

Output



```
def piab(q, params):
```

User defines the probability density

Python

Example

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User defines how to run the MC sampling

```
q = MATRIX(1,1);  q.set(0, 0.5)
params = {"k":1.0, "m":2000.0, "states":[0], "coeffs":[1.0]}
Nsamp = 1000000; Nstart = 50000
sampling = metropolis_gau(rnd, HO_sup, q, params, Nsamp,Nstart, 0.05)
bin(sampling, -1.5, 2.0, 0.01, 0, 0, "_distrib-1.txt")
```

User defines what probability distribution function is to be sampled

```
def HO_sup(q, params):
    k = params["k"];    m = params["m"];
    states = params["states"];    coeffs = params["coeffs"]
    x = q.get(0)
    sz = len(states)
    p = 0.0
    for n in xrange(sz):
        p = p + coeffs[n] * ket_n(x, states[n], k, m)
    p = p * p
    return p
```

The dynamical algorithm is in C++, but…

Don’t need to implement the model in C++

Initial Conditions: Metropolis Sampling

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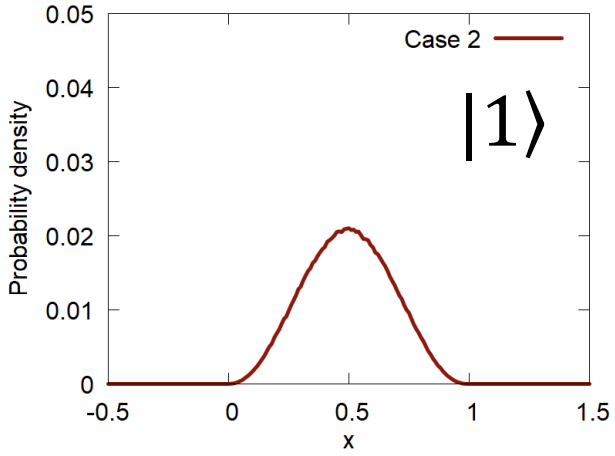
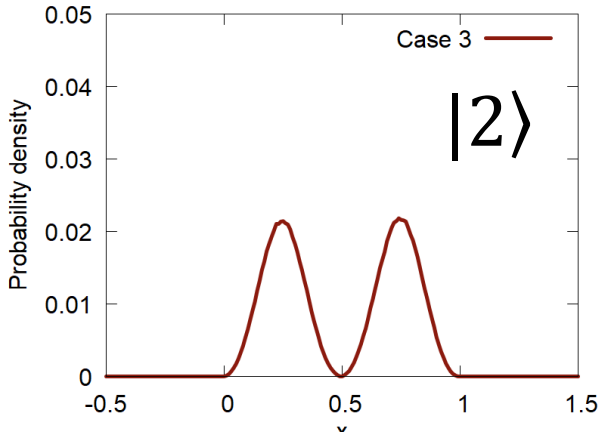
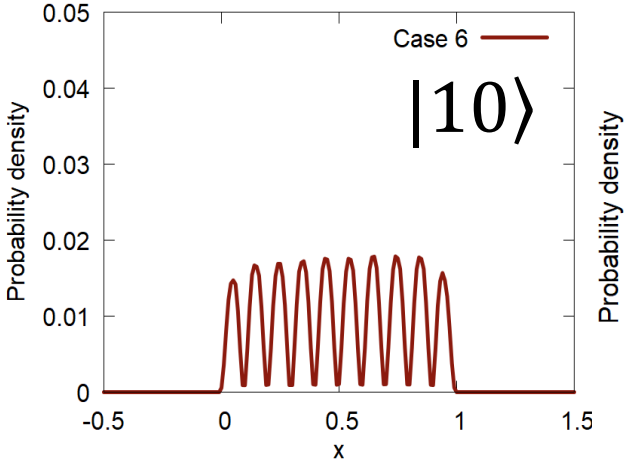
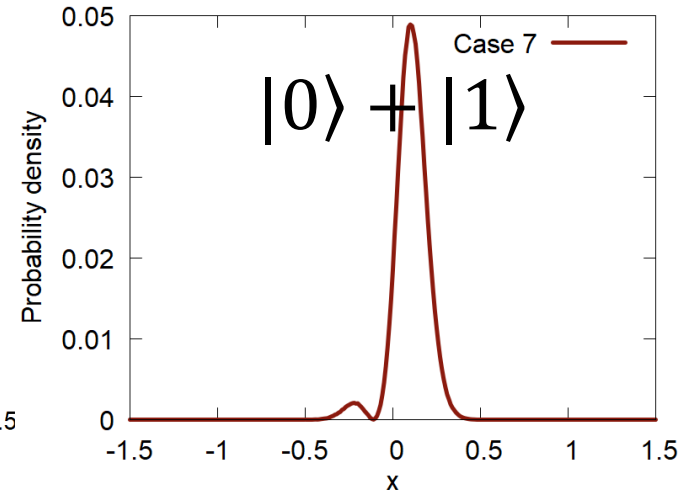
Particle in a box

$$\psi_n(q) \sim \sin\left(\frac{\pi n q}{L}\right)$$



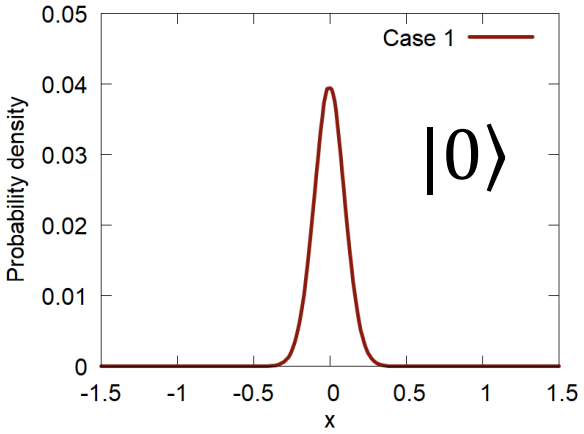


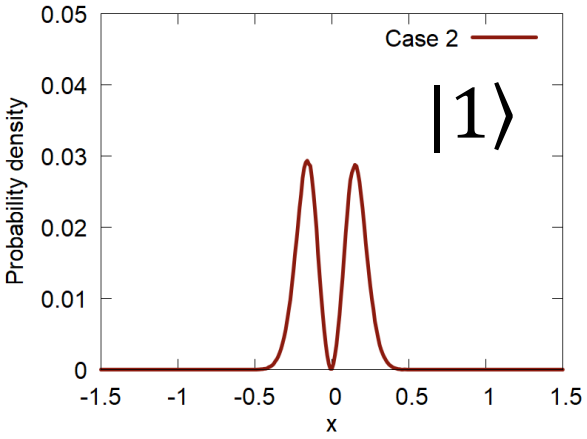


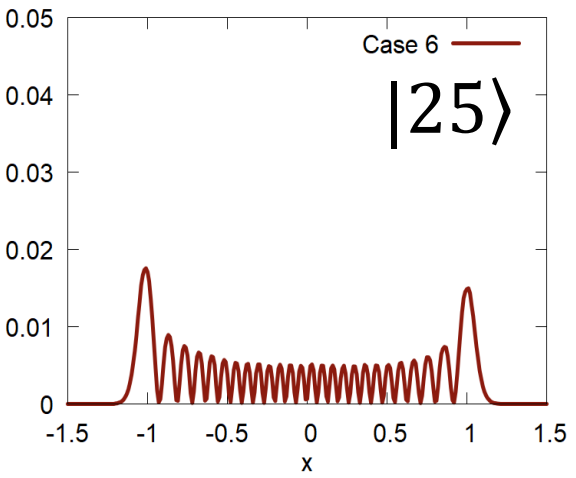


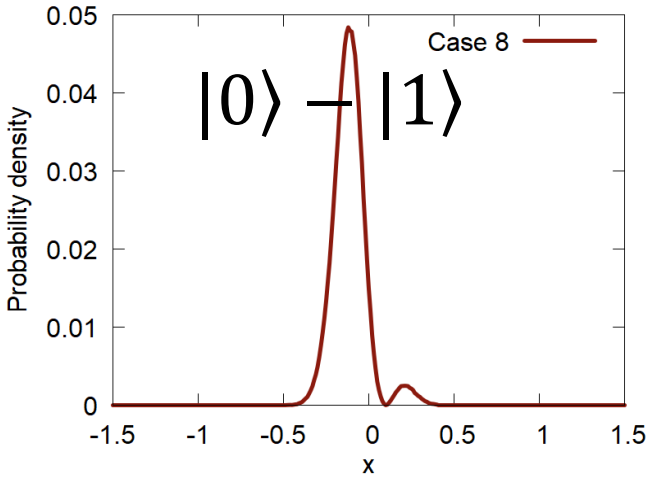
Harmonic oscillator

$$\psi_n(q) \sim H_n(q\sqrt{\alpha}) \exp\left(-\frac{\alpha q^2}{2}\right)$$









Why 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 best standards and facilitate bug discovery/testing

How to Contribute?

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The State University of New York

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

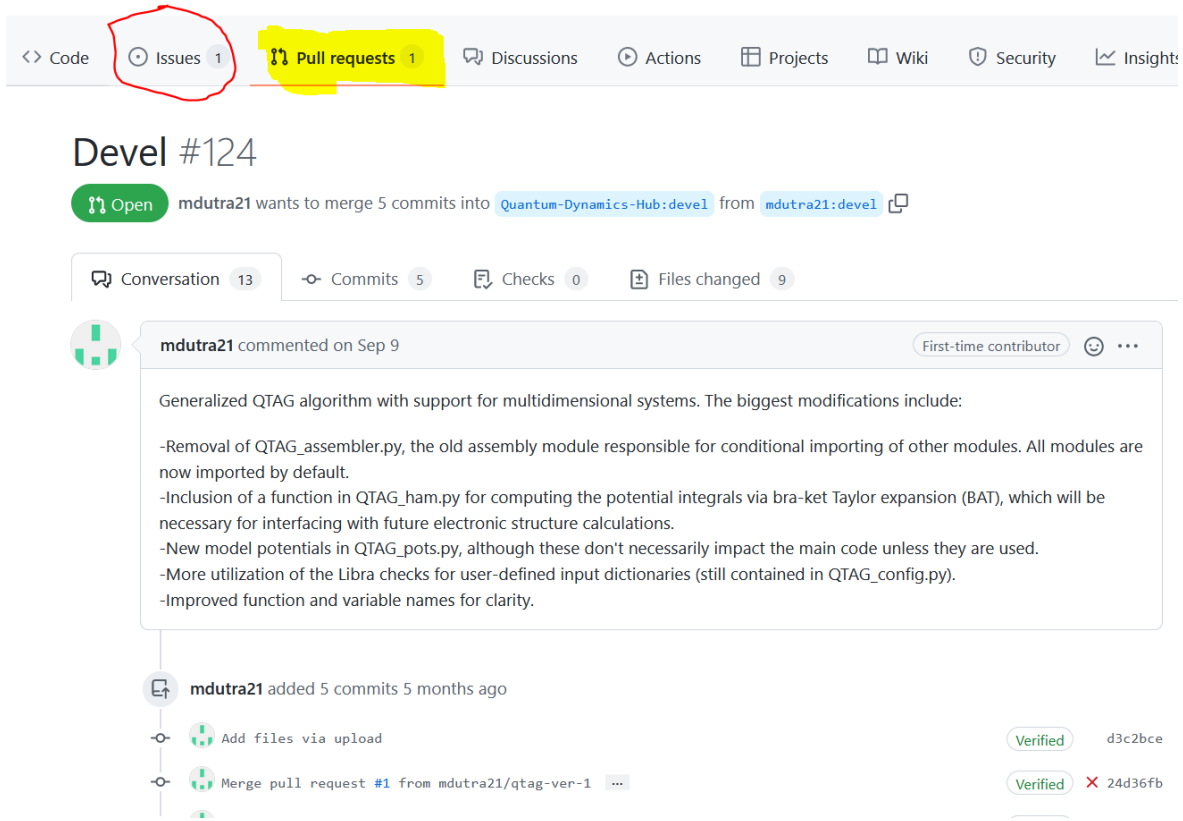
https://github.com/amber-jain-group-iitb/heom_amber

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)