

Machine-Learning in Quantum and Nonadiabatic Dynamics



Home

Agenda

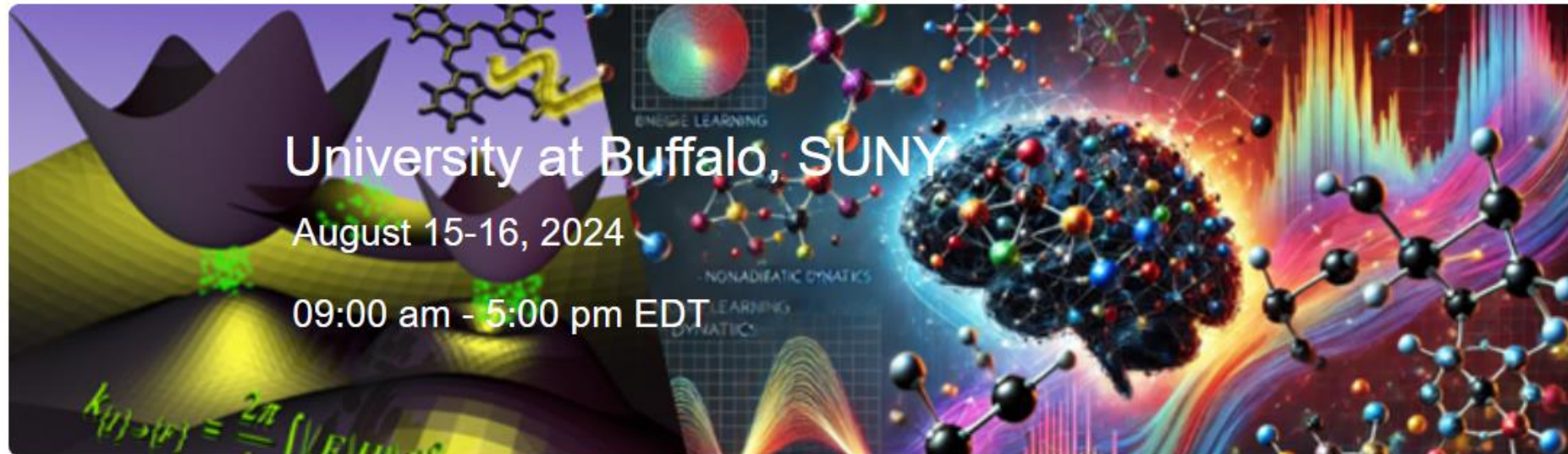
Resources

Setup

Episodes ▾

Extras ▾

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(Credit: Mohammad Shakiba & ChatGPT)

https://quantum-dynamics-hub.github.io/MolSSI_workshop2024/

University at Buffalo, SUNY, Aug 15-16, 2024

Objectives of this Workshop



Daniel Crawford – director of **MolSSI**

Objectives:

- **Awareness:** learn about the **new/best practices** of using ML in electronic structure, quantum dynamics, and related simulations
- **Interdisciplinary cross-pollination:** focus on different closely- or more distantly-related fields – look for common usages, know-hows, and potential problems; share and discuss ideas; educate each other;
- **Software motivation!!!:** learn about **practical aspects (codes, software, tutorials)** of such calculations – one of MolSSI's mission. Try to be practical.

Working Plan

Hybrid format: in-person + Zoom

Join Slack:

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

**Please provide
your input:**

Google Docs:

<https://docs.google.com/document/d/1D8pYIUbMmg3Nx45jb6nTULSxjGsXQsdsf0jxeMc07tY/edit?usp=sharing>

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

* Please use the #molssi-2024 channel

WeChat: ???

Work in small groups in the breaks – also remote participants

The summary of the working documents will be made available on the Website

Lectures will be videorecorded, abstracts and presentations will be made available via the Website

Organizers and Helpers



Alexey Akimov



Daeho Han



Mohammad Shakiba



Qingxin Zhang

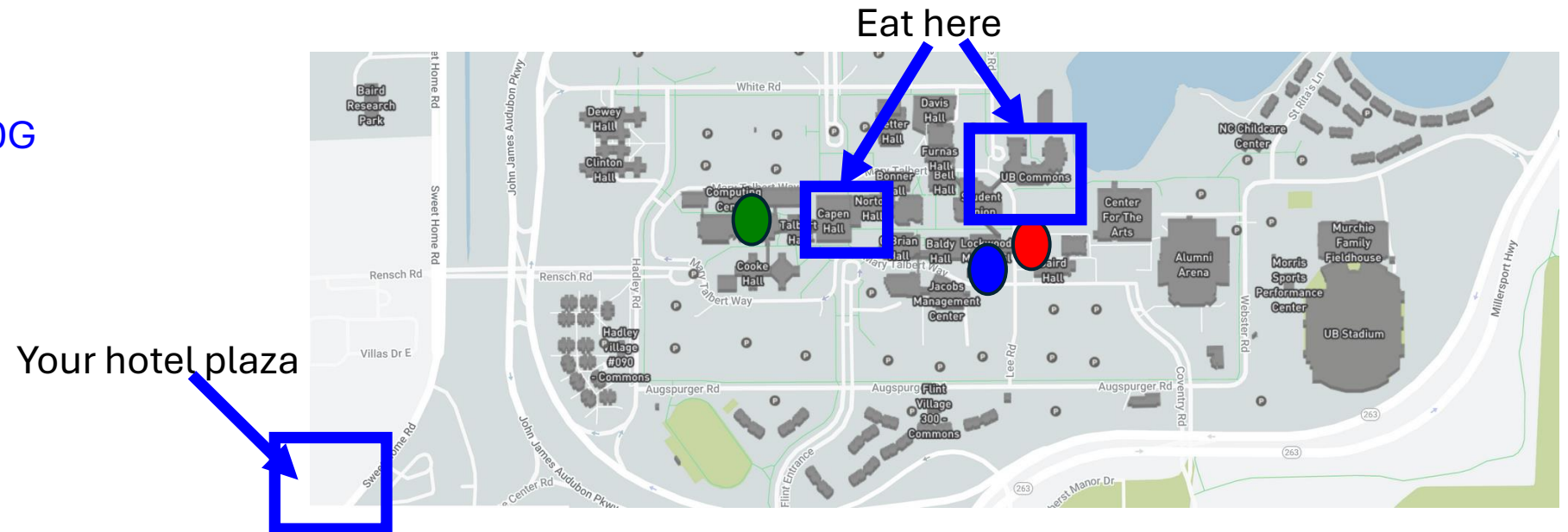
Daily Schedule

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” or “World Cafe”, 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

- Aug. 15 – Baldy Hall 200G
- Aug. 16– Clemens 120



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