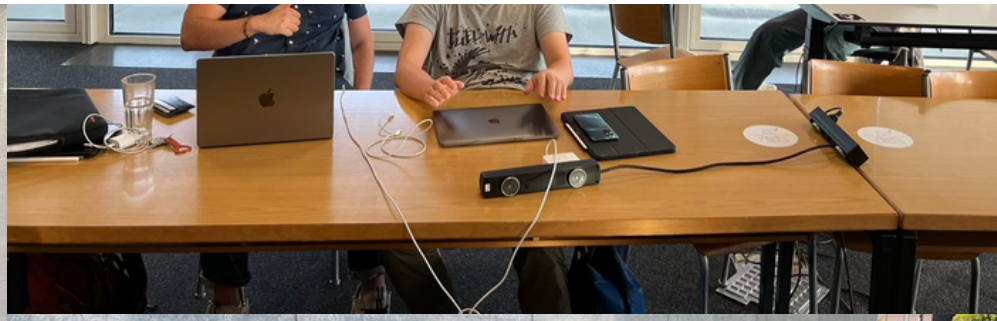
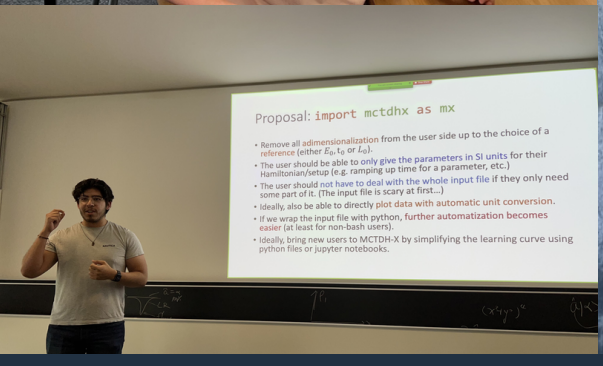
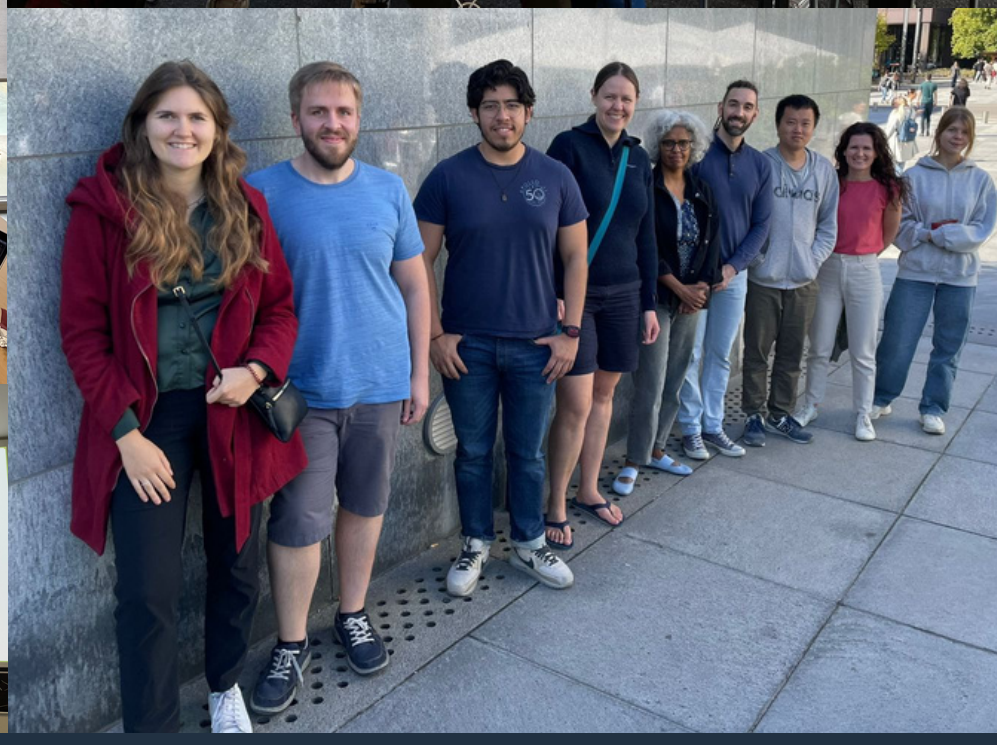
Software Developer Workshop for the Numerical Simulation of Ultracold Quantum Many-Body Systems

Unitary Fund Microgrant Project

Zürich, Switzerland, October 2023







Abstract from applicaton

The MCTDH-X software solves the time-dependent many-body Schrödinger equation for quantum particles. It surpasses mean-field simulations of ultracold systems for ground-state physics and dynamics. Applications span fundamental research (e.g. new phases of matter) to quantum advantage (e.g. benchmarking quantum simulators) with over 50 publications to date. The MCTDH-X team is organizing a workshop to form the next generation of code maintainers, merge all branches into an integrated, user-friendly version, expand its capabilities to simulate more complex setups, e.g. ultracold atoms coupled to fully quantum gauge/light fields. The updated, handier code will facilitate guidance in cutting-edge experiments in ultracold labs, e.g. at ETH Zurich and University of Hamburg, advancing established collaboration. It will be promoted in the quantum network (online workshops or conferences e.g. in Heidelberg in July 2023) to expand the user-base and engage a new wave of young quantum scientists.

Introducing our team

Participants of the workshop:
In the group picture, from left to right:

- Manuel Eder, Master student, Institute of Physical and Theoretical Chemsitry, University of Tübingen, Germany
- PD Dr. Ramasubramanian Chitra, P.D., Institute for Theoretical Physics, ETH Zurich, Switzerland
- Elke Fasshauer, Junior Research Group Leader, Institute of Physical and Theoretical Chemsitry, University of Tübingen, Germany; *(also affiliated with:)* Department of Chemistry, University of Oxford, United Kingdom
- Rui Lin, Postdoc, Institute for Quantum Optics and Quantum Information (Innsbruck), Austrian Academy of Sciences, Austria
- (only visiting for 1 day:) Elena Jahr, PhD student, Institute of Physical and Theoretical Chemsitry, University of Tübingen, Germany
- Miriam Büttner, PhD student, Institute of Physics, University of Freiburg, Germany
- Lydia M. Fichte, Master student, Institute of Physical and Theoretical Chemsitry, University of Tübingen, Germany
- Paolo Molignini, Postdoc, Department of Physics, Stockholm University, Sweden
- Yuliya Bilinskaya, Master student, Department of Physics, Stockholm University, Sweden
- Daniel A. Ortuño González, Master student, Institute for Theoretical Physics, ETH Zurich, Switzerland

Not in the group picture, but participating remotely:

- Sunayana Dutta, Postdoc, Research Center for Theoretical Physics & Astrophysics, University of Haifa, Israel
- Rhombik Roy, Postdoc, Research Center for Theoretical Physics & Astrophysics, University of Haifa, Israel
- (only giving a talk:) Ofir E. Alon, Prof., Research Center for Theoretical Physics & Astrophysics, University of Haifa, Israel
- (for daily Q&A sessions:) Axel U.J. Lode, former senior MCTDH-X developer, Freiburg, Germany

Goals of the workshop & schedule

Broadly speaking, the developer workshop was intended to get the code and its newest users up to speed. And to eventually release a new version that is more user friendly and includes the developments of the past couple of years.

The MCTDH-X code was first released around 10 years ago. Since then, a number of individual theoretical physicists and chemists have contributed to it by adding new features, but the documentation of the various new features has often been too sporadic. That has made both development and external use and application increasingly more difficult in the past years.
Our current research and development objectives include bosons or fermions in optical cavities that are being subjected to external lasers, the dynamics of trapped dipolar molecules, the simulation of rotating Bose-Einstein Condensates and the simulation of bosonic Josephson junctions. These objectives are being pursued in academic groups in currently 5 different countries and the respective implementations live of different branches on GitLab.

So to be more specific about the goals of the workshop: On the one hand, we wanted to advance the aforementioned research objectives by fostering discussions between people that work on different projects but with related routines in the code and in doing so avoid implementation chaos, and on the other hand we wanted to merge all the different branches from the different groups into the main branch and add documentation to it.

The overview schedule was:

monday	tuesday	wednesday	thursday	friday
presentation day	2 more presentations	continue w/ yesterday's focus groups	potentially continue w/ focus groups	wrap up and discuss results
Q&A w/ senior developer	Q&A w/ senior developer	new focus groups	invited speaker	
	work in 3 separate focus groups	discuss results	new focus groups	
			workshop dinner	

A more detailed schedule can be provided if necessary.
On the next page we have added a bit more detail to what the topics of the talks were and what the focus groups were. A discussion of what was achieved can be found on the subsequent page.

from Monday, Oct 9th 2023: discussions and mingling in between presentations

Talk Topics during the Workshop

- Introduction to MCTDH-X theory: The equations of motion
- Understanding the core routines: Visualizing the call structure with doxygen
- The Cavity+BEC module and what we can do with it
- New addition to the software: Rotating Bose-Einstein-Condensates
- Automated input file and python wrapper for MCTDH-X
- Quantum simulators with dipolar molecules and Quasicrystals
- How accurate is MCTDH-X: Computing fidelities (through equal-time overlaps, unequal-time overlaps or overlaps from different bases), autocorrelation functions and Loschmidt echos in MCTDH-X
- Convergence: What is required and how we ensure it

from Monday, Oct 9th 2023:
Daniel giving his talk on the automated input file and python wrapper he is developing for MCTDH-X users that are unfamiliar with Fortran

Focus Groups during the Workshop

- Merging (Miriam, Elke, Sunayana)
- Fidelity (Yuliya, Manuel, Rhombik)
- Domain-decmposed orbitals and MPI (Rui, Daniel, Paolo, Axel)
- Spinor systems (Paolo, Elke, Lydia, Chitra, Karin)
- Fermionic cavity (Paolo, Elke, Lydia, Chitra)
- Tutorial paper (Paolo, Elke)
- Code documentation (Miriam)
- Unit testing (Paolo, Elke, Axel)
- Updating installation + guide (Rui, Miriam)

code longevity
user friendliness
extension
extension
extension
user friendliness
code longevity
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user friendliness

from Tuesday, Oct 10th 2023:
three focus groups at work. depcited here are (from left to right) the focus groups “Domain-decmposed orbitals and MPI”, “Fidelity” and “Merging”.

Achievements of the workshop

from Thursday, Oct 12th 2023: participants happy at the end of the day

As a result of the talks:

- Overview of science performed with the code
- Onboarding new developers
  - Code structure
  - Questions to be answered with this code
  - Familiarize with parts of the code
- Software Management
  - Best practices using version control with git
  - Merging developments into main branch
  - Discussions about testing strategy
  - Development and benchmarking of parallelization with MPI
  - First dummy test implemented (real test have to follow)
- Strategic discussions for further development

As a result of the focus groups:

- Merging:
  - merged branches with recent developments and deleted some stale branches
  - documented purpose of old and stale branches that might still be useful in the future
  - decided on introducing version numbers for our public releases for more accountability, clearer testing of backward compatibility from the developers' perspective and better replicability of published results from the users' perspective
- Fidelity:
  - revised implementation (bugs and confusing standard output)
  - started writing new section in the user manual explaining all the types of fidelity/autocorrelation functions/overlap that the code can do
- Domain-decmposed orbitals and MPI:
  - enabled benchmarking of core functionalities in both relaxation (imaginary time propagation) and (real-time) propagation
  - for relaxation mode: tested MPI implementation taking both the one-body interaction and the two-body interaction into account (specifically contact interaction and the gaussian interaction)
  - for propagation mode: tested MPI implementation with only one-body interactions
- Spinor systems:
  - Initiated project for new master student. She will be in charge of benchmarking MCTDH-X for fermions with spins (spin ½). This is part of the bigger plan to provide more functionalities and stability for simulations with fermionic systems.

- Fermionic cavity (Paolo, Elke, Lydia, Chitra):
  - discussed how to extend the cavity module to deal with particles with internal degrees of freedom and in particular spinful fermions (the spinless fermionic and bosonic codes are working fine already)
  - plans for funding for a new PhD student specifically for this were made
- Tutorial paper (Paolo, Elke):
  - new MCTDH-X Tutorial paper to be published soon in IOP's Journal of Physics B
- Code documentation (Miriam):
  - decided on style guide for code documentation
  - made code documentation accessible not only for developers and doxygen users, but for everyone through GitLab pages website
- Unit testing (Paolo, Elke, Axel):
  - first tried "Funit" framework, but decided against it because it does not seem to be compatible with the way the code is structured (intricate module co-dependencies)
  - Instead decided on CTest which is a part of CMake, because MCTDH-X is already compiled via CMake
  - wrote first test, but still much to do
- Updating installation + guide (Rui, Miriam):
  - fixed issues in installation guide that led to multiple users having to ask for help on our discord server
  - installation guide and manual are now separate

from Thursday, Oct 12th 2023: the Domain-decmposed orbitals and MPI benchmarking finally worked

Left to do:

We want to put a new public release out (with version number) that includes our updated code and the extended manual. We want to make it easier for users to navigate, so the additions to the manual should be in there, as well as the Python wrapper for the input and our website needs to still be updated accordingly.

We would be happy about suggestions from the side of the Unitary Fund team, regarding what else people in the community might want to see as part of our software, since the goal always was to contribute to the quantum community as best we can.