

SIMPLAIX workshop: Machine learning for multiscale molecular modeling



Molecular mechanisms and the rational design of molecules and materials for specific applications have traditionally been explored using physics-based modeling and simulations. These methods have revolutionized modern science and technology. However, they reach their limits when it comes to mapping, exploring, and analyzing the infinitely complex and variable structures and properties of molecular systems over the wide range of relevant scales. Here, data-driven and machine learning methods offer a promising approach. This is why HITS, Heidelberg University, and the Karlsruhe Institute of Technology (KIT) launched the SIMPLAIX collaboration in fall 2021. They aim to combine the expertise of the three partner institutions, focusing on

bridging scales in simulating biomolecules and molecular materials by multiscale simulation and machine learning. SIMPLAIX is coordinated by HITS researchers **Rebecca Wade** and **Frauke Gräter**. The initiative is enabled by the Klaus Tschira Foundation and financially supported by the three institutions. Young researchers have been recruited to work in the 8 subprojects. To date, 7 internal project meetings have been organized in Heidelberg and Karlsruhe, and several joint HITS-SIMPLAIX colloquium talks were given, on topics related to neural networks, computational chemistry and atomistic-scale modeling. “SIMPLAIX has enabled us to collaborate on interdisciplinary, interinstitutional research projects,” says Rebecca Wade, who serves as spokesperson of the collaboration. “By combining machine learning and simulation approaches, we expect to gain novel insights into scale-bridging molecular phenomena in complex biomolecules and molecular materials that will ultimately lead to new approaches to molecular design.”



The next step is an international SIMPLAIX workshop on “Machine Learning for Multiscale Molecular Modeling.” It will take place at the HITS conference venue, the Studio Villa Bosch in Heidelberg, on 2-4 May 2023. The Workshop will bring together scientists working in the field to share their research and discuss current challenges. 14 distinguished speakers from Europe, Asia and North America will cover a wide range of topics. The workshop is designed to enable informal presentations and discussions, with a focus on the interaction between senior and young researchers.



Via Data
The HITS blog can be found on the “Scilog” portal at <https://scilog.spektrum.de/via-data/>.

HITS

Astronomy and climate crisis: HITSters win outreach competition

How can research be made accessible and tangible for everyone? To answer this question, students and researchers took part in the university competition organized by Wissenschaft im Dialog (WiD). The Year of Science 2023’s theme is “Our Universe.” 76 entries communicating ideas about the “Universe” were submitted. Only 15 were selected, among them a concept by HITSters **Eva Laplace, Dandan Wei, Duresa Temaj, Vincent Bronner, Rajika Kuruwita, Julian**



Saling (all SET) and **Jan Henneco** (SET and TOS): a board game called “Habitable” that links astronomy with the climate crisis by motivating players to create a habitable

planet where life is possible despite changing conditions. “We are all big fans of board games,” says Eva Laplace, “and we wanted families and friends to enjoy a fun game that inspires its players to think about climate change, the habitability of our planet and humankind’s impact on it.” The researchers will receive funding of 10,000 euros to implement their idea.

New employees and visiting scientists

- Senior Researcher:** Melanie Schienle (CST)
Postdoc: Debora Monego (MBM), Sebastian Trujillo Gomez (AIN)
Research Associates: Alexandra Kozyreva (PSO), Gerhard Mayer (SDBV)
Pre-docs: Tommaso Bartoloni (MCM), Mislav Brajkovic (MCM), Alessandro Calzolari (CCC), Dominique Ostermayer (CCC, HITS Lab)
Visiting scientist: Angeliki Papadopoulou, Hellenic Republic University of Crete
Communications: Ida Bahmann
Administration: Harald Haas (Controlling)

HITS groups (03/2023): *Astroinformatics (AIN), Computational Carbon Chemistry (CCC), Computational Molecular Evolution (CME), Computational Statistics (CST), Data Mining and Uncertainty Quantification (DMQ), Groups and Geometry (GRG), Machine Learning and Artificial Intelligence (MLI), Molecular Biomechanics (MBM), Molecular and Cellular Modeling (MCM), Natural Language Processing (NLP), Physics of Stellar Objects (PSO), Scientific Databases and Visualization (SDBV), Stellar Evolution Theory (SET), Theory and Observations of Stars (TOS).*

HITSters

Surfing the research data wave

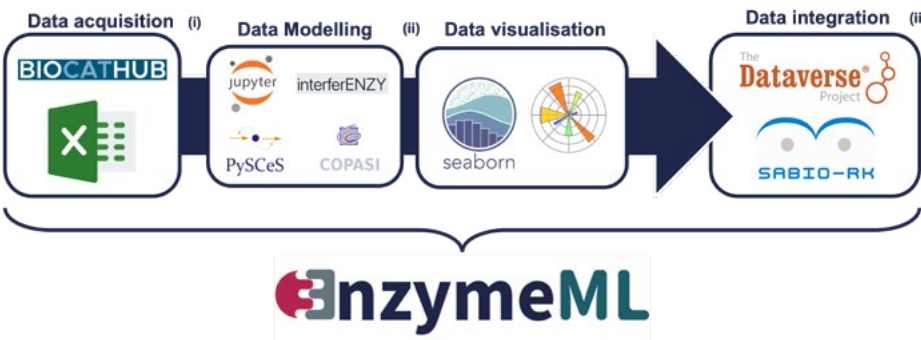


While more and more data is generated by an increasing number of researchers and increasing research expenditure world-wide, this data is hardly manageable by our scholarly practice of communicating scientific results. The lack of standards, incomplete metadata, and missing original data make it nearly impossible to reproduce published results.

This also applies to studies on the catalytic activity, selectivity and stability of enzymes and enzymatic networks, a field of research that is equally important for industrial biotechnology and biomedicine. Moreover, data describing enzymatic experiments is particularly complex, because an enzymatic reaction depends on many factors, such as the protein sequence of the enzyme, or the pH value. The new, standardized data exchange

format “EnzymeML,” presented by 23 authors from 14 different research institutions in the scientific journal “Nature Methods” gives hope in this respect. EnzymeML can completely record the results of an enzymatic experiment, from the reaction conditions to the measured data, as well as the kinetic model used to analyze experimental data and the estimated kinetic parameters.

The format thus provides a seamless communication channel between experimental platforms, electronic lab notebooks, enzyme kinetics modeling tools, publication platforms, and enzymatic reaction databases.



HITS researchers **Ulrike Wittig** and **Andreas Weidemann** (Scientific Databases and Visualization) are in charge of the data integration in EnzymeML. They use SABIO-RK, a reaction kinetics database developed at HITS, where the kinetic data will be stored directly after they have been modeled.

Simone Lauterbach et al.: EnzymeML: “Seamless data flow and modeling of enzymatic data”, Nature Methods 2023, DOI 10.1038/s41592-022-01763-1 <https://www.nature.com/articles/s41592-022-01763-1>

Research

Beyond the limits: Sarbani Basu, Klaus Tschira Guest Professor



“It’s almost like being a postdoc again,” says **Sarbani Basu**, sitting at the desk of her office that is looking on to the garden. “This is a fantastic program.” The sun research specialist and former chair of the department of astronomy at Yale University, Connecticut (USA) is the second Klaus Tschira Guest Professor at HITS, and spent more than two months at the institute, from mid-September to late November 2022.

The Klaus Tschira Guest Professorship Program aims to enhance international exchange and scientific collaboration at HITS. Internationally renowned scientists are invited for sabbaticals or extended research stays. They collaborate with scientists at HITS, develop joint research projects, and engage with the wider scientific community at the institute and in the Heidelberg region. In 2023, HITS will host another two Klaus Tschira Guest Professors. Sarbani Basu used her stay to mainly collaborate with the “Theory and Observations of Stars” (TOS) research group led by **Saskia Hekker**. “I have known Saskia for quite a long time and started working with her when she was a postdoc in Birmingham”, she recalls. “Here at HITS, I am working with her and her group on a long-time project about the interior structure of stars. I hope we will be ready to publish some results in a year’s time.” Moreover, she is collaborating with TOS postdoc **Felix Ahlborn** on the rotations inside the stars.

“For this, he will use the inversion technique I had developed, and which he enhanced, to investigate these rotations,” she explains.

During her stay, she gave a HITS colloquium talk on the physics of the sun in early October, and delivered further talks at Heidelberg, as well as at the joint colloquium series of the Max Planck Institute for Astrophysics (MPA), the Max Planck Institute for Extraterrestrial Physics (MPE) and the European Southern Observatory (ESO) in Garching. She also enjoyed the opportunity to engage in discussions with scientists from other scientific disciplines at HITS, for example in the coffee bar or on her daily commute on the “Science Bus” that connects the HITS campus to the city.

In the course of her fellowship, the collaboration with Saskia Hekker gained momentum. “We can continue with it remotely when I am back in the U.S.,” Sarbani Basu says. “After six years of running the department of astronomy at Yale, being completely away helped me to start thinking about science again.” And she adds: “This program is an amazing opportunity to sit down and just concentrate on science.”

Imprint | Dr. Peter Saueressig (Vi.S.d.P.), saueressig@h-its.org, Tel. +49 6221 533 245 | Pictures: HITS, EnzymeML | www.h-its.org

Beyond the limits



The charts