Digital Laboratory for Mathematics in Chemistry

Funded by the Foundation for Innovation in University Teaching, we want to develop the Digital Laboratory Mathematics for Chemistry from 2025.

The project aims to teach chemistry students basic mathematical and programming skills that are essential for understanding chemical concepts. This includes topics such as differential and integral calculus, exponential and logarithmic functions, differential equations and Fourier transforms, which are used in chemical applications such as thermodynamics, reaction kinetics and spectroscopy. Instead of learning these mathematical concepts in the abstract, they apply them directly to chemical problems by carrying out computer experiments and writing their own code.

Jupyter notebooks are set up for computer experiments. They offer an interactive and flexible environment that facilitates the introduction to programming and also enables visualisations. The notebooks help to link mathematical and chemical content and to learn modern digital tools for analysing data. The level of difficulty of the tasks can be adjusted very easily in the range from pure presentation to challenging tasks. It is therefore comparatively easy to respond to different requirements and to adapt the materials created for related courses, for example.

The project is being developed in co-operation with various universities in German-speaking countries. Through these co-operations, a wide range of teaching and research experience flows into the design of the computer experiments. Hackathons already organised for the joint development of teaching material have been very successful in this context. As the project is scheduled to run for four semesters, we have the opportunity to take student feedback into account and incorporate it into the development process. This ensures that the experiments remain practical and are continuously improved.



Participants in the teaching hackathon in summer semester 2024, with cooperation partners from the research groups Römelt (HU Berlin), Bahmann (Uni Wuppertal), Stein (TU München), Keller (FU Berlin), Stopkowicz (Uni Saarland), Lear (Penn State College). Also insolved are the research groups Podewitz (TU Wien) and Proppe (TU Braunschweig).