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Lab@Home: Individualised computer-lab courses

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Abstract

Die im Jahr 2020 aufgetretene Pandemie bedingte auch an den Universitäten einen Lockdown und die Verlagerung der Lehre in den digitalen Raum. Im Bereich der Studiengänge Chemie und Lebensmittelchemie ist dies nur teilweise möglich. Insbesondere die Laborpraktika vermitteln Kernkompetenzen, die nicht anders als in Präsenz erworben werden können. Computerpraktika hingegen können mit guter Konzeption an den heimischen Computer verlagert werden. Wir stellen hier unser Konzept vor, das es möglich gemacht hat, Computerversuche aus den Bereichen der Quantenchemie und Statistischen Thermodynamik als Lab@Home-Computerpraktikum durchzuführen. Individualisierte Aufgabenstellung, kontrollierte Vorproduktion der numerischen Ergebnisse, fortlaufende Kommunikation mit den Studierenden und umfangreiche Nutzung digitaler Lehrmethoden waren dabei die entscheidenden Grundlagen für die erfolgreiche Durchführung.

The pandemic that occurred in 2020 also caused a lockdown at universities and the relocation of teaching to the digital space. In the area of the Chemistry and Food Chemistry degree programmes, this is only partially possible. The laboratory courses in particular convey core skills that cannot be acquired in any other way than in presence. Computer-lab courses, on the other hand, can be relocated to the home computer with a good underlying concept. We present our concept here, which has made it possible to conduct computer experiments from the fields of quantum chemistry and statistical thermodynamics as Lab@Home computer-lab courses. Individualised tasks, controlled pre-production of numerical results, continuous communication with the students and extensive use of digital teaching methods were the decisive foundations for successful implementation.

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1. Introduction

Part of the training in the Chemistry and Food Chemistry degree programmes deals with the subject of theoretical chemistry. This part teaches the basics of quantum mechanics, various models for calculating molecular properties as well as methods of electronic-structure calculations. Due to the interdisciplinary nature of this field, students are confronted with problems from physics, mathematics and computer applications, all of which are required to deal with chemical problems. We have made the experience that teaching these interdisciplinary subjects through practical exercises (hands-on courses) works well. Therefore, we designed, carried out, and improved corresponding computer experiments already years ago [1].

Usually, this computer lab took place under supervision at fixed time slots in a well-equipped computer pool. However, due to the pandemic that occurred in 2020 and the resulting lockdowns, attendance courses were not feasible at all or only under difficult circumstances. We therefore decided at an early stage to move this part of our courses to the digital space: as Lab@Home. We benefited from the fact that nowadays all students are equipped with computer hardware and we do not have to conduct practical experiments in the laboratory.

In this article, we present our concept of transferring these computer experiments into individualised experiments that can be conducted in the home office. The planning for the summer semester 2020 was done within two weeks after presence teaching at TU Dresden was shut down. We have constantly developed our concept ever since, which now is running successfully for the second year, and adapted it to individual circumstances of different courses.

2. Computer-lab courses

We have applied our present concept to two computer-lab courses in the Bachelor Chemistry and Food Chemistry degree programmes. Both computer labs are integrated into the physical chemistry (PC) module canon and will be described here briefly: Module PC2 ("Theory of Chemical Bonding") takes place as a compulsory module of both degree programmes in the third semester and deals with the basics of quantum mechanics (Schrödinger equation, particle in a box, harmonic oscillator, hydrogen atom, molecular-orbital theory, Hückel theory) as well as basics of electronic-structure calculations, e.g. Hartree-Fock method and density-functional theory. In addition to the lecture and a seminar series, the content is mainly taught in the PC2 computer lab, which includes five computer experiments. Their topics are: (1) atomic orbitals, (2) ionisation potential, (3) molecular-orbital theory, (4) Hückel theory, and (5) vibrational spectroscopy.

In the sixth semester, students of the Bachelor's degree programme in Chemistry also take part in the compulsory module PC3 ("Special Physical Chemistry"), which deals with photochemistry, electrochemistry, theoretical chemistry, and statistical thermodynamics. In addition to the lectures and a series of seminars, a lab course has to be attended. It consists of two equal parts: a practical laboratory course covering the areas of photochemistry and electrochemistry, and a part with computer experiments dealing with theoretical chemistry and statistical thermodynamics.

For both computer labs (PC2, PC3), the same rules apply: Each of the five (PC2) or three (PC3) experiments is introduced in advance by a topic-related seminar, in which the most important basics are revisited and special features of the experiment are discussed. Afterwards, students have the opportunity to take an electronic test over a period of four days in order to be admitted to the computer experiment. The grade achieved here is entering the final grade. There are two options of repetition for this test within the specified period. Table 1 summarises important parameters of both computer labs.

The computer experiment takes place on a fixed date in the faculty's computer pool, where 20 workstations are equipped with the necessary software. Each experiment is carried out in groups of two, the results are discussed and reported in writing, and the lab report is handed in at the end of the day. The time required for the students on site is about four hours per experiment if they are well prepared.

Tab. 1: Summary of important characteristics of the two modules in which Lab@Home computer labs were carried out. The duration refers to those semesters with Lab@Home mode.

	Module PC2	Module PC3
Module title	Theory of Chemical Bonding	Special Physical Chemistry
Study programmes	Chemistry, Food Chemistry	Chemistry
Students	approx. 90 (approx. 45 groups of two)	approx. 40
Semester	3rd (winter semester)	6th (summer semester)
Number of experiments	5 (+ pre-experiment)	3 (+ pre-experiment)
Duration	13 weeks	8 weeks

3. Challenges

The start of a lockdown of uncertain duration in spring 2020 made a decision necessary whether and how the PC3 computer lab could be carried out that was scheduled for the summer semester. In particular, the uncertainty about the lockdown duration quickly led us to the decision to move the computer lab to the digital space and the students' homes. As a consequence, the lockdown could be used already and reserved time slots were made available to colleagues that had to carry out experimental lab courses. This solution was very well received by both our students and colleagues.

Since the teaching quality had to be guaranteed even under these exceptional conditions, the relocation of the computer lab to the students' homes as a virtual Lab@Home course raised a number of questions that had to be solved in advance:

- Is the applied computational-chemistry software suitable for use by inexperienced students without direct supervision?
- How can we guarantee the correct and fast software installation on different hardware with different operating systems?
- How can we prevent disadvantages for individual students due to underperforming hardware?
- How can we guarantee asynchronous yet continuous supervision while the computer experiments are being carried out?
- How can we make all students deal with the material themselves and carry out the necessary steps independently?
- How can we construct electronic tests that are taken at home, but still monitor the students' performances in a meaningful way?

4. Approach: Lab@Home

Our approach to solving these questions was to individualise the Lab@Home computer lab. In this section we first explain the individual solutions to the questions raised in the previous section, and in the following section we give an overview of the modalities of the Lab@Home that have emerged after three semesters.

The computational-chemistry software used in the computer lab was the ADF (Amsterdam Density Functional) software package even before the pandemic [2,3]. Teaching licences can be negotiated with many computational-chemistry software companies. This programme has a graphical user interface, where molecules can be generated intuitively and all parameters of the calculation to be performed can be chosen in drop-down menus (Fig. 1). Since this software runs on the common operating systems (MS Windows, Mac OS, Linux), it was ideally suited for our approach. We accompany the installation process and operation through a messenger service channel, but also by email and, if necessary, by video conferencing. In general, no major problems arise here, as the installation process of this commercially available software is already optimised for the three common operating systems.

In addition to the Lab@Home option, however, we also keep two fully equipped desktop workstations in individual offices on the campus, so that students without the necessary hardware requirements could carry out the experiments at any time under the necessary precautions. In this way, we achieve a barrier-free computer lab.

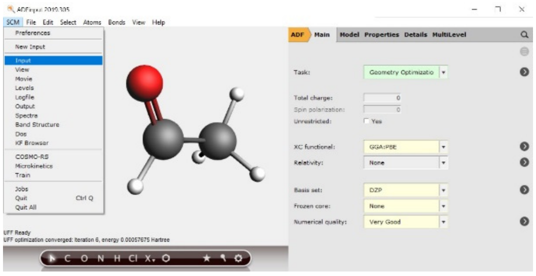
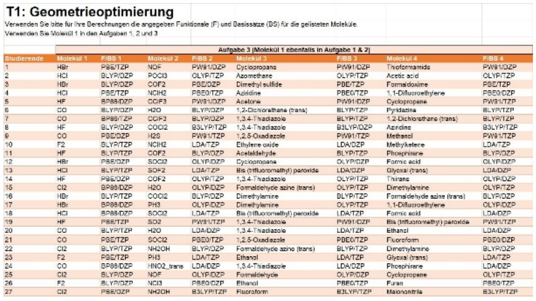


Fig. 1: Graphical user interface of the ADF programme package [2,3]. Molecules can be created intuitively and calculation parameters can be set in various drop-down menus.

The installation of the software is accompanied by a preliminary experiment, for which no report has to be handed in. In adition to the installation instructions, the students receive the numerical results of certain calculations in order to reproduce them and, thus, get familiar with the software handling. Additionally, we ask for the required computing time. This gives us an estimate of the individual hardware, and a sensible assignment of the calculation parameters can be made. Students with less powerful hardware work on data sets that are less demanding in terms of computational resources.

For asynchronous yet continuous support of the computer experiments, we use the messenger service [matrix] [4] which is well-established at TU Dresden. The respective computer-lab chat channel for questions and advice is supervised for approx. 12 hours per day, both on weekdays and weekends, so that the students do not lose time while working on the experiments. The staff of the Chair of Theoretical Chemistry is involved here and takes turns in providing support.

The biggest challenge was quality assurance: While in a computer pool the balancing between desired instructive exchange among students and undesired sharing of solutions can be monitored relatively easily, this is no longer possible in a Lab@Home situation. We were able to circumvent this problem by individualising the tasks: The students were assigned individual calculation parameters and molecules to be investigated. Thus, the same results are obtained qualitatively, but they differ quantitatively (Fig. 2).



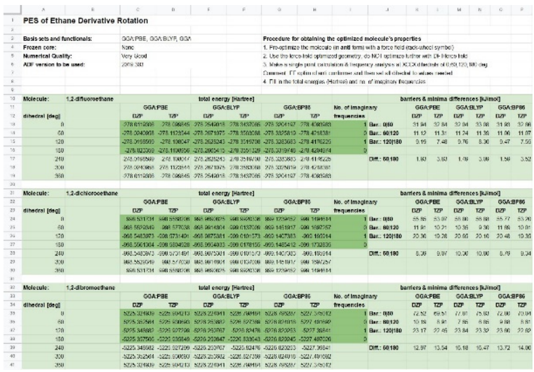
T1: Geometrieoptimierung

Verwenden Sie bitte für Ihre Berechnungen die angegeben Funktionale (F) und Basissätze (BS) für die gelisteten Moleküle.
Verwenden Sie Molekül 1 in den Aufgaben 1, 2 und 3

	Aufgabe 3 (Molekül 1 ebenfalls in Aufgabe 1 & 2)							
Studierende	Molekül 1	F/BS 1	Molekül 2	F/BS 2	Molekül 3	F/BS 3	Molekül 4	F/BS 4
1	HBr	PBE/TZP	NOF	PW91/DZP	Cyclopropane	PW91/DZP	Thioformamide	PW91/DZP
2	HCl	BLYP/DZP	POCl3	OLYP/TZP	Azomethane	OLYP/TZP	Acetic acid	OLYP/TZP
3	HBr	BLYP/DZP	COF2	PBE/DZP	Dimethyl sulfide	PBE/TZP	Formaldoxime	PBE/TZP
4	HCl	PBE/TZP	NClH2	PBE0/TZP	Aziridine	PBE0/TZP	1,1-Difluoroethylene	PBE0/DZP
5	HF	BP86/DZP	CClF3	PW91/DZP	Acetone	PW91/DZP	Cyclopropene	PW91/TZP
6	CO	BLYP/DZP	H2O	BLYP/DZP	1,2-Dichlorethane (trans)	BLYP/TZP	Pyridazine	BLYP/TZP
7	CO	BP86/TZP	CClF3	BLYP/DZP	1,3,4-Thiadiazole	BLYP/TZP	1,2-Dichlorethane (trans)	BLYP/TZP
8	HF	BLYP/DZP	COCl2	B3LYP/TZP	1,3,4-Thiadiazole	B3LYP/DZP	Aziridine	B3LYP/TZP
9	CO	PBE/DZP	H2S	PW91/TZP	1,2,5-Oxadiazole	PW91/TZP	Methanol	PW91/TZP
10	F2	BLYP/TZP	NClH2	LDA/TZP	Ethylene oxide	LDA/DZP	Methylketene	LDA/TZP
11	HF	BLYP/TZP	COF2	BLYP/DZP	Acetaldehyde	BLYP/TZP	Phosphirane	BLYP/DZP
12	HBr	PBE/DZP	SOCl2	OLYP/DZP	Cyclopropane	OLYP/DZP	Formic acid	OLYP/DZP
13	HCl	BLYP/TZP	SOF2	LDA/TZP	Bis (trifluoromethyl) peroxide	LDA/DZP	Glyoxal (trans)	LDA/DZP
14	HF	PBE/DZP	COF2	OLYP/TZP	1,3,4-Thiadiazole	OLYP/TZP	Thirane	OLYP/DZP
15	Cl2	BP86/DZP	H2O	OLYP/DZP	Formaldehyde azine (trans)	OLYP/TZP	Dimethylamine	OLYP/TZP
16	HBr	BLYP/TZP	COCl2	BLYP/DZP	Dimethylamine	BLYP/TZP	Formaldehyde azine (trans)	BLYP/DZP
17	HBr	BP86/DZP	PH3	OLYP/DZP	Dimethylamine	OLYP/TZP	1,1-Difluoroethylene	OLYP/DZP
18	HCl	BP86/DZP	SOCl2	LDA/TZP	Bis (trifluoromethyl) peroxide	LDA/TZP	Formic acid	LDA/DZP
19	HF	PBE/TZP	SO2	PW91/TZP	1,3,4-Thiadiazole	PW91/DZP	Bis (trifluoromethyl) peroxide	PW91/TZP
20	CO	BLYP/TZP	H2O	LDA/DZP	1,3,4-Thiadiazole	LDA/TZP	Ethanol	LDA/DZP
21	CO	PBE/TZP	SOCl2	PBE0/TZP	1,2,5-Oxadiazole	PBE0/TZP	Fluoroform	PBE0/DZP
22	Cl2	BLYP/TZP	NH2OH	BLYP/DZP	Formaldehyde azine (trans)	BLYP/TZP	Dimethylamine	BLYP/DZP
23	F2	PBE/TZP	PH3	LDA/TZP	Ethanol	LDA/TZP	Glyoxal (trans)	LDA/TZP
24	CO	BP86/DZP	HNO2_trans	LDA/DZP	1,3,4-Thiadiazole	LDA/DZP	Phosphirane	LDA/DZP
25	Cl2	BLYP/DZP	NOF	OLYP/DZP	Formaldehyde	OLYP/DZP	Cyclopropene	OLYP/TZP
26	F2	BLYP/DZP	NCl3	PBE0/DZP	Ethanol	PBE0/TZP	Furan	PBE0/TZP
27	Cl2	PBE/DZP	NH2OH	B3LYP/TZP	Fluoroform	B3LYP/TZP	Malononitrile	B3LYP/TZP

Fig. 2: Individual assignment of different molecules and calculation parameters (functionals, basis sets) to the students.

In this way, the fundaments for the didactically desired conclusions could be laid, but the corresponding calculations had to be carried out independently by all participants, i.e. individual results had to be produced. Thus, solving the tasks independently was encouraged and copying of results was made more difficult. This approach proved to be very successful. In addition, all results produced by the students were checked in advance, so that the discussion in the reports was not carried out with results that were incorrect in content.



PES of Ethane Derivative Rotation

Fig. 3: Example of a shared spreadsheet filled in by the Theoretical Chemistry staff. Each calculation was carried out independently by two persons in order to avoid errors.

Of course, individualisation entails a considerable amount of extra work in advance, because all individual data sets had to be produced and checked first. This was not only necessary as a basis for report checking, but also served to filter out didactically unfavourable combinations of molecules and/or calculation parameters. In practice, this pre-production of results was implemented by the members of the Chair of Theoretical Chemistry, who compiled and checked the results in shared spreadsheets (Fig. 3) from their home offices. In total, several thousand data sets were produced in this way.

While the controlled individualisation of the computer lab led to independent engagement with the material, joint tasks initiated constructive cooperation between the students. For example, students contributed to the temperature-dependent plot of an isomer distribution in a shared spreadsheet, with each participant contributing a pair of values (Fig. 4). The resulting graph was then discussed in the reports. From the evolving solution, the students could also assess whether or not they were correct with their results.

New tasks covering current topics were developed to draw the students' interest beyond their normal occupation with the subject. This seemed particularly important in a home office situation, where also direct exchange among students is reduced. In the third semester (module PC2), the molecular basics of the greenhouse effect were included in an experiment. Thereby, the purpose was solely about teaching the physicochemical basics, i.e. scientifically understood processes. Understanding these gives all students the opportunity to form their own opinion in the political debate on the basis of scientific principles.

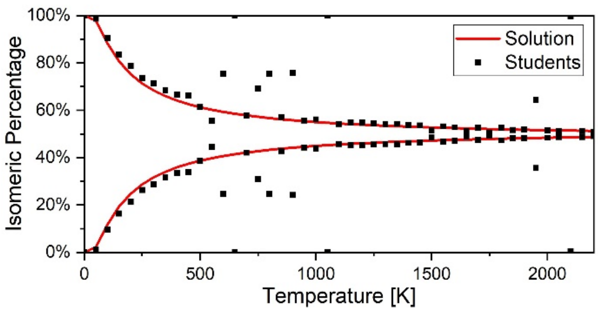


Fig. 4: Diagram created from the shared spreadsheet in which students entered their results. The two red curves show the correct result, the black dots the students' individual results with some deviations.

The communication with students was performed electronically only. The reports were written electronically and submitted via upload, either in groups of two (module PC2) or alone (module PC3).

Finally, a satisfactory solution had to be found to replace the entrance tests. Originally, they serve to reduce the teaching effort on the lab day, because only well-prepared students can learn from the computer experiments and perform them in the available time slot. By moving the experiments to the home office completely, this was no longer required. At the latest, the students learned the matter during carrying out the experiments. Students with sufficient previous knowledge were able to complete the tasks faster than unprepared participants. We therefore converted each entrance test into an exit test in order to check and reward learning success.

To summarise, the challenges of moving the computer labs to the students' homes can be addressed as follows:

- Software suitability: The ADF programme package is well suited to the demands of a Lab@Home situation. Other software may also be suitable; however, we did not test any. It is recommended to pay attention to simple installation procedures and intuitive usability. The possibility of purchasing teaching licences or free licensing is certainly an advantage.
- Correct installation: Even though commercial programmes are usually designed to be installed reliably, we have accompanied the installation procedure with a pre-experiment.
- Technical equality: The individual computing times for given tasks indicated the hardware performance. We took this into account, when assigning the individual data sets.
- Asynchronous yet continuous support: Messenger services offer optimal response times to questions.
- Independence: The individualisation of the tasks leads to independent engagement with the subject. Joint tasks provide additional motivation.
- Exit instead of entrance tests: To check and reward learning success, electronic exit

tests were carried out, that entered the grades.

5. Digital support

Use of a learning platform: The advantages of using a learning platform became apparent latest with the beginning pandemic. We had already used the local Saxonian learning platform OPAL intensively for teaching purposes before. The following features were particularly helpful:

- Student registration: e-mail communication with students was possible at any time.
- Upload/download folders: The digital reports were submitted by the students via upload. The corrected and graded reports were made available for download afterwards.
- Electronic tests: The exit tests were carried out using the test tool ONYX . No retake option was given for exit tests. In a few cases, the experiment was concluded with an oral exam.
- Forum: Initially, the learning platform's integrated forum was used to answer questions. However, the messenger service has proven to be more suitable for this purpose.
- Exams: During the pandemic, all final exams were conducted online with individualised problems and tasks.

Synchronous/asynchronous digital lectures: All module lectures were recorded and could be accessed online throughout the semester via a video platform (Videocampus Sachsen [5]) of the local Saxony Education Portal [6]. It was, thus, possible to maintain the classic lecture format with 90 minutes of front-of-class teaching, because the lectures could be viewed in full or partly if required. The lectures were either recorded from the lecture hall with some students being present or from the lecturer's laptop via video streaming.

Online seminars with breakout sessions: Keeping the participants' attention during seminars was one of the biggest challenges, as these were not recorded for various reasons. This was mainly done by interrupting the lecturer's talk by breakout sessions where students could work on tasks in randomly generated small groups. Partly, the tasks were related to the computer experiments. This created variety throughout a 90 minutes course and encouraged independent engagement in the subject. The psychological barrier for asking questions was significantly reduced in small groups.

Educational videos: In addition to digital seminars, the essential contents of the computer experiments were summarised in short educational videos to provide the students with studying material in different formats. Two to three videos per experiment were produced, each of 10 to 20 minutes length. The videos were published via the local video platform Videocampus Sachsen.

Digital exam: Setting up a digital exam was certainly one of the biggest challenges. While the technical prerequisites were given by the local learning platform OPAL and the test tool ONYX, it mainly was a matter of a good conception of exam questions. We decided on an open-book exam (including internet use), since the use of unauthorised aids could not be controlled in any way under the given circumstances. The questions were adapted accordingly, so that an internet search for answers would not yield any usable results in the given time. In addition, the assignments were individualised as well and randomly distributed and sorted. Communication among the students, which could not be ruled out in general, would take too much time and could be reduced to a minimum. In summary, the grades' distribution did not differ from those of previous years, though the failure rate slightly increased.

Communication: Communication with the students proved to be a decisive point for the success of the computer lab. Here, a quick response to questions seemed to be important. As a consequence we switched from using a forum to using a messenger service, as the message notification function seemed implemented technically better.

The term communication also included giving students the feeling of being looked after: Additionally to publishing all deadlines, modalities and computer-experiment educational material well in advance, we also sent out weekly e-mails each Friday with all events, deadlines and further information for the upcoming week.

7. Lab@Home key points

For the successful implementation of a Lab@Home computer-lab course, the following points have emerged for us as being crucial:

- Individualisable tasks (quantitatively different, qualitatively analogous).
- Good and continuous electronic communication with students.
- Asynchronicity through provided educational videos and lecture recordings.
- Conducting electronic tests, also as preparation for digital exams.
- Willingness of the responsible personnel for new and unusual teaching and evaluation formats.

These points require more staff and time, both in preparation and in implementation. We have estimated that the effort per semester is around 1,000 man-hours, but probably even higher. This number does not include the time needed for conception. A well-coordinated, not too small team is therefore absolutely necessary.

In upcoming semesters, the effort will certainly decrease, but the numerical results regularly must be checked for consistency after software updates.

8. Sustainability and diversity

Computer-lab courses generally can be regarded as a sustainable form of teaching. Individual studies of the course material is performed without the use of chemicals and even independently of the available computer-pool space on campus. The individualisation entailed an increased preparation and supervision effort, as several thousand data sets had to be produced and tested in advance. This process can be at least partially automated by experienced team members using scripting languages. However, the data sets have to be checked for consistency as soon as software updates are carried out. Generally, however, the data sets are available for further years. They can also be used for future courses taught in presence. Although these will be synchronous courses, the material for each participating group still can be individually assigned.

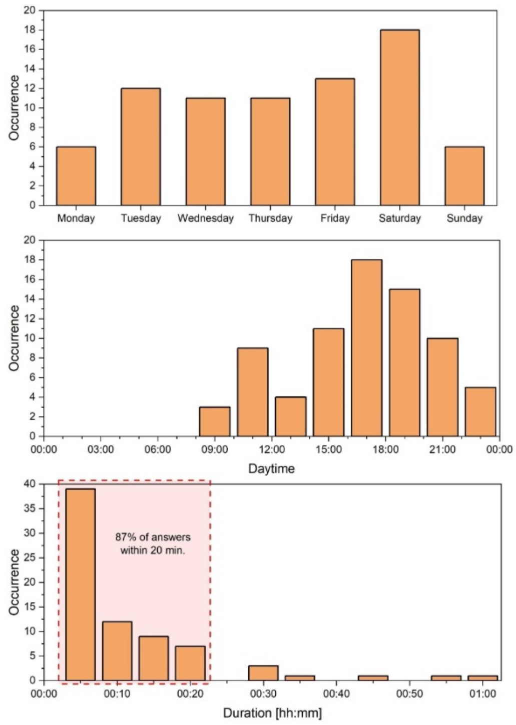


Fig. 5: Statistical evaluation of the activities of the messenger service channel for winter semester 2020/21: Question frequency by weekday (top) and time of day (middle) as well as response time by our staff (bottom).

In particular, the statistical evaluation of the computer-lab channel in the messenger service [matrix] showed that the work habits of the students strongly changed compared to a typical daily routine with on-campus teaching (Fig. 5). The Lab@Home tasks increasingly were carried out at the weekend and in the evenings. The statistics also show that our staff managed to answer about 90% of the questions within 20 minutes, regardless of day or time.

For students in exceptional circumstances, as e.g. illness or absence, the option of completing an asynchronous computer lab is certainly attractive. With the simultaneous offer of doing it on campus site (through provided, bookable hardware in the campus area), our

Lab@Home computer courses are truely barrier-free.

9. Summary and outlook

Due to the 2020 pandemic and the resulting university lockdowns, we were forced to develop a new concept for all our computer-lab courses. In the meantime, Lab@Home courses are running successfully for three semesters already. The most important challenge during the lab-course development was maintaining the teaching quality. We have achieved this by individualising the assignments. In addition, we have ensured good and continuous communication with the students. Here, a messenger service proved to be beneficial. In this way, it was possible to give the students, who were dealing with the studying material alone, a feeling of support. The possibility of asynchronous learning and barrier-free accessibility were particularly well received by the participants. In addition to the course subjects, the students had to deal with computer-technical issues (programme installation, advanced use of spreadsheet programming etc.), from which they will benefit as well.

Acknowledgement

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