

Please note that this English version of the study and examination regulations is nothing more than an aid to orientation. Solely the German version is legally binding.

Study and examination regulations for the joint Master's program Computational Sciences of the Department of Biology, Chemistry, Pharmacy, the Department of Earth Sciences, the Department of Mathematics and Computer Science and the Department of Physics at the Freie Universität Berlin

Preamble

On the basis of Section 14 paragraph 1 no. 2 of the Partial University Constitution (Trial version) of the Freie Universität Berlin of 27 October 1998 (FU Mitteilungen [Gazette of the Freie Universität Berlin] 24/1998), the Joint Commission for the joint Master's program Computational Sciences of the Department of Biology, Chemistry, Pharmacy, the Department of Earth Sciences, the Department of Mathematics and Computer Science and the Department of Physics issued the following study and examination regulations for the joint Master's program Computational Sciences of the Department of Biology, Chemistry, Pharmacy, the Department of Earth Sciences, the Department of Mathematics and Computer Science and the Department of Physics at the Freie Universität Berlin on 21 January 2016:¹

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¹ The executive board of the Freie Universität Berlin confirmed these regulations on 09 February 2016.

Section 1 Area of Applicability

(1) These regulations apply to the aims, content and structure of joint Master's program Computational Sciences of the Department of Biology, Chemistry, Pharmacy, the Department of Earth Sciences, the Department of Mathematics and Computer Science and the Department of Physics at the Freie Universität Berlin (Master's program) and the requirements and procedures for achieving the study and examination attainments (attainments) on the Master's program as a supplement to the Framework Study and Examination Regulations of the Freie Universität Berlin (RSPO).

(2) This is a consecutive Master's program in accordance with Section 23 paragraph 3 No. 1 part a) of the law regulating higher education institutions in Berlin (Berlin Higher Education Act – BerlHG) of 26 July 2011 (Law and Ordinance Gazette (GVBl) p. 378). The program structure is research-focused.

Section 2 Qualification objectives

(1) Graduates of the Master's program have mastered a wide range of terminology, structures, techniques and methods in the modern computer-aided natural sciences. They are able to work independently to formalize even complex applied scientific issues in mathematical terms, can structure the resulting mathematical problems and prepare them for computer-aided solutions, select appropriate solution methods and apply them or implement them independently and communicate their findings in lectures or texts.

(2) Graduates of the program have gained skills in scientific research, in reading and writing scientific texts in the English language and in lecture and presentation techniques. They have a modern approach to gender and diversity issues and have gained skills in teamwork, communication and knowledge transfer.

(3) Thanks to their general ability to identify abstract connections in complex problems, to bring together terminology and structures from applied science and mathematics and to apply these to solving problems, graduates of the Master's program are not restricted to a defined professional field. A range of areas of business, science, administration and industry present opportunities for future careers.

Section 3 Program content

(1) The Master's program covers fundamental and advanced terminology, structures, methods and processes in a wide range of structured and applied areas of scientific knowledge combined with supplementary courses. It ensures that students have the opportunity to specialize in current research and promotes the development of independent scientific thinking with a particular focus on the use of computers to expand knowledge.

(2) Students gain and deepen their competence in combined mathematical, computer-related and applied scientific expertise, as well as systematically developing their interdisciplinary skills and key qualifications. By preparing lectures and reports, students learn to present their expertise and qualifications orally or in writing in a suitable form in relation to their audience. They learn to deal with gender and diversity issues in practicals and practice groups and through supervising tutorials. For example, the students learn to take cultural differences into account when working in the participating departments' research groups, which are usually international in composition.

Section 4 Academic advisory center and departmental advisory service

(1) General student advisory services are provided by the center for academic advising and psychological counselling of the Freie Universität Berlin.

(2) The departmental advisory service is provided by the professors who run the courses on the Master's program during their regular office hours.

(3) We urgently recommend students to make an appointment for a consultation with the chairperson of the examination committee or their deputy within the first two weeks of the first semester. This consultation should cover the individual's program plan, in particular the plan for the Synchronization area, the Scientific Computing area, and the focus of their Specialization area. Sufficient appointments for this purpose are provided and announced in good time in a suitable way.

Section 5 Examination committee

The examination committee appointed by the Joint Commission for the joint Master's program Computational Sciences of the Department of Biology, Chemistry, Pharmacy, the Department of Earth Sciences, the Department of Mathematics and Computer Science and the Department of Physics at the Freie Universität Berlin is responsible for organizing the examinations and other tasks listed in the RSPO.

Section 6 Regular duration of study

The regular duration of study is four semesters.

Section 7 Structure and organization; scope of attainments

(1) A total of 120 credit points (CP) must be attained in the Master's program. The Master's program is structured as follows:

1. Synchronization area comprising 30 CP
2. Scientific Computing area comprising 30 CP
3. Specialization area comprising 30 CP
4. Master's thesis with accompanying colloquium comprising 30 CP.

(2) The Synchronization area comprising 30 CP provides students from different subject-based backgrounds with supplementary skills in other subjects to complete their expertise profile. The Synchronization area offers the following discipline-related modules:

- a) Chemistry
 - Module: Introduction to Molecular Spectroscopy (5 CP)
 - Module: Introduction to Theoretical Chemistry (5 CP)
 - Module: Quantum Mechanical Description of Atoms and Chemical Bonding (10 CP)
- b) Geographical Sciences
 - Module: Principles of Remote Sensing and Digital Image Analysis (5 CP)
 - Module: Principles of Hydrogeography and Climate Geography (5 CP)
 - Module: Principles of Geographical Information Systems (5 CP)
- c) Geological Sciences
 - Module: Synchronization Earth (10 CP)
- d) Computer Science
 - Module: Complex Algorithms A (15 CP).
 - Module: Computer Science and Data Structures A (15 CP)
 - Module: Computer Science and Functional Programming A (15 CP)
 - Module: Computer Science and Object-Oriented Programming A (15 CP)
- e) Mathematics
 - Module: Introduction to Numerical Mathematics A (15 CP),

- Module: Numerics of ODEs and numerical linear algebra A (15 CP)
- Module: Numerics of partial differential equations A (15 CP)
- Module: Synchronization Mathematics (15 CP)

f) Meteorology

- Module: Atmospheric Dynamics (8 CP)
- Module: Introduction to Atmospheric Dynamics (7 CP)
- Module: Principles of Synoptic Meteorology (7 CP)

g) Physics

- Module: Computational Statistical Physics I A (15 CP)
- Module: Computational Statistical Physics II A (15 CP)
- Module: Introduction to Quantum Mechanics (10 CP)

In the Synchronization area, the Computational Sciences module (15 CP) is obligatory. Modules totaling 15 CP are also to be taken as follows, depending on each student's previous knowledge:

1. Students with a Bachelor degree in Chemistry, Geographical Sciences or Geological Sciences with the module sequence Principles of Natural Sciences focusing on Chemistry and Biology must take the following module:

- Module: Synchronization Mathematics (15 CP).

2. Students with a Bachelor degree in Mathematics, Computer Science or Engineering Sciences must select and complete modules totaling 15 CP from the following subject areas as listed in clause 2 above:

- Chemistry
- Geographical Sciences
- Geological Sciences
- Meteorology
- Physics

3. Students with a Bachelor degree in Physics must select and complete modules totaling 15 CP from the following subject areas as listed in clause 2 above:

- Geographical Sciences
- Geological Sciences
- Computer Sciences
- Mathematics
- Meteorology

4. Students with a Bachelor degree in Meteorology must select and complete modules totaling 15 CP from the following subject areas as listed in clause 2 above:

- Chemistry
- Geographical Sciences
- Geological Sciences
- Computer Sciences
- Mathematics
- Physics

5. Students with a Bachelor degree in Geological Sciences with the module sequence Principles of Natural Sciences focusing on Mathematics and Physics must select and complete modules totaling 15 CP from the following subject areas as listed in clause 2 above:

- Chemistry
- Informatics
- Mathematics
- Meteorology
- Physics

(3) In the Scientific Computing area, two modules totaling 30 CP must be selected and completed. One module from each of Variant A and Variant B must be selected. Students may not select the same module from Variant A and B.

1. The following modules are offered in Computer Science:

- Module: Complex Algorithms A (15 CP) or
Module: Complex Algorithms B (15 CP),
- Module: Computer Science and Data Structures A (15 CP) or
Module: Computer Science and Data Structures B (15 CP),
- Module: Computer Science and Functional Programming A (15 CP) or
Module: Computer Science and Functional Programming B (15 CP),
- Module: Computer Science and Object-Oriented Programming A (15 CP) or
Module: Computer Science and Object-Oriented Programming B (15 CP).

2. The following modules are offered in Numerics:

- Module: Introduction to Numerical Mathematics A (15 CP) or
Module: Introduction to Numerical Mathematics B (15 CP),
- Module: Numerics of ODEs and numerical linear algebra A (15 CP) or
Module: Numerics of ODEs and numerical linear algebra B (15 CP),
- Module: Numerics of partial differential equations A (15 CP) or
Module: Numerics of partial differential equations B (15 CP).

3. The following modules are offered in Statistics:

- Module: Computational Statistical Physics I A (15 CP) or
Module: Computational Statistical Physics I B (15 CP),
- Module: Computational Statistical Physics II A (15 CP) or
Module: Computational Statistical Physics II B (15 CP)

(4) The Specialization area totaling 30 CP may be selected from these three areas: Molecular Sciences, Geosciences und Atmospheric Sciences. Students are to select a specialization area from among these three options by the start of the 2nd semester and are to register their choice with the examination committee. Not more than one Research Project module (A to E) in total may be selected. In individual cases, students may be permitted to take modules from other Master's programs at the Freie Universität Berlin or other universities for the Specialization area on application to the examination committee, on condition that the students gain admission to these modules. Selecting modules from different specialization areas is not possible.

1. Specialization area Molecular Sciences:

a) Required modules: the following modules totaling 10 CP must be completed:

- Module: Molecular Simulation I (5 CP) and
- Module: Quantum Chemistry (5 CP).

b) Compulsory elective modules: Modules totaling 20 CP must be selected from the following module list and completed:

- Module: Density Functional Theory (5 CP)
- Module: Research Project A (5 CP) or
Module: Research Project E (10 CP)
- Module: Research Seminar computational sciences (5 CP)
- Module: Markov Modeling (5 CP)
- Module: Molecular Simulation II (5 CP)
- Module: Quantum Chemical Correlation Methods (5 CP)
- Module: Quantum Reaction Dynamics (5 CP)
- Module: Selected topics in applied computational sciences (5 CP) and/or
- Module: Selected topics in theoretical computational sciences (5 CP)

For information on the modules Quantum Chemistry (5 CP), Density Functional Theory (5 CP), Quantum Chemical Correlation Methods (5 CP) and Quantum Reaction Dynamics (5 CP), students are referred to the Study and Examination Regulations for the Master's program Chemistry of the Department of Biology, Chemistry, Pharmacy at the Freie Universität Berlin.

2. Specialization area Geosciences:

a) Required modules: the following modules totaling 12 CP must be completed:

- Module: Geophysics I (6 CP) and
- Module: Seismics II (6 CP).

b) Compulsory elective modules: Modules totaling 18 CP must be selected from the following modules and completed:

- Module: Earth Dynamics (6 CP)
- Module: Research Project A (5 CP) or
Module: Research Project C (7 CP)
- Module: Research Seminar computational sciences (5 CP)
- Module: Geophysics II (6 CP)
- Module: Selected topics in applied computational sciences (5 CP)
- Module: Selected topics in theoretical computational sciences (5 CP) and/or
- Module: Thermodynamics und Kinetics of Geological Processes (6 CP).

For information on the modules Geophysics I (6 CP), Seismics II (6 CP), Earth Dynamics (6 CP), Geophysics II (6 CP) and Thermodynamics und Kinetics of Geological Processes (6 CP) students are referred to the Study and Examination Regulations for the Master's program Geological Sciences of the Department of Earth Sciences at the Freie Universität Berlin.

3. Specialization area Atmospheric Sciences:

a) Required module: The following module totaling 8 CP must be completed:

- Module: Weather and Climate Diagnosis (8 CP)

b) Compulsory elective modules: Modules totaling 22 CP must be selected from the following module list and completed:

- Module: Research Project B (6 CP) or
Module: Research Project D (9 CP)
- Module: Research Seminar computational sciences (5 CP)
- Module: Climate Variability and Climate Models (8 CP)
Module: Models for Weather and the Environment (8 CP)
- Module: Satellite Meteorology (8 CP)
- Module: Selected topics in applied computational sciences (5 CP)
- Module: Selected topics in theoretical computational sciences (5 CP)
- Module: Theoretical Meteorology I (8 CP) and/or
Module: Theoretical Meteorology II (8 CP).

For information on the modules Weather and Climate Diagnosis (8 CP), Climate Variability and Climate Models (8 CP), Models for Weather and the Environment (8 CP), Satellite Meteorology (8 CP), Theoretical Meteorology I (8 CP) und Theoretical Meteorology II (8 CP) students are referred to the Study and Examination Regulations for the Master's program Meteorology of the Department of Earth Sciences at the Freie Universität Berlin.

(5) Information about the modules for the Master's program, covering admissions requirements, content, qualification objectives, types of teaching and learning units, workload hours, forms of active participation, the examination attainments required during the course, information on compulsory regular attendance at the teaching and learning units, credit points allocated to the modules, regular duration and how often the module is offered is given in the module descriptions in Annex 1.

(6) Information about the recommended study plan for the Master's program is given in the sample study schedule in Annex 2.

(7) Students may not select modules from the list of elective modules in paragraphs 2 to 4 that are identical to modules already completed in their Bachelor program. In doubtful cases the examination committee will take a decision on this matter; the decision is to be taken before the relevant module is completed.

Section 8

Teaching and learning units

(1) The following types of teaching and learning units are provided in the Master's program:

1. Lecture (L): Lectures cover the theoretical principles of the topic focused on in each case, teach theories and methods of analysis and critically examine the current state of the computer sciences.
2. Introductory course (IC): Introductory courses are designed to give an introduction or cover basic principles. The main type of teaching unit is a lecture by the course lecturer in on-site classes and talks and discussions moderated by the lecturer on fundamental topics, problems or issues.
3. Seminar (S): Seminars aim to examine methodological issues and offer a critical approach to possible applications and application fields.
4. Project seminar (PS): Project seminars aim to examine a sample topic area in detail and give the chance to practice independent scientific work. Guided by an lecturer, students apply what they have learnt to a concrete computer science problem in the form of a project. The findings are prepared, presented and discussed. The proportion of independent work by the students is greater than in seminars.
5. Laboratory practical (LaP): Laboratory practicals enable the practical application of the students' new knowledge and methodological skills in the field of laboratory methods.
6. Practical (P): Practicals enable students to work independently on issues and possible solutions on selected objects using appropriate methods and to learn practical manual and analytical skills.
7. Practice seminar (PracS): Practice seminars are intended to convey working techniques, practical knowledge or computer skills.
8. Seminar on the computer (SPC): Seminars on the computer provide practice and in-depth learning of theoretical content using computer simulations.

(2) The teaching and learning units as listed in paragraph 1 may be implemented using Blended Learning arrangements. This entails on-site classes linked to electronic internet-based media (e-learning). Selected teaching and learning activities are provided via the Freie Universität Berlin's central e-learning application so that students can work on them singly or in groups, either independently or under supervision. Blended learning can be applied in the implementation phase (exchange and discussions of learning objects, problem-solving, increasing the communication between students and lecturers) or in the follow-up phase (monitoring learning progress, promoting knowledge transfer).

Section 9 Master's thesis

- (1) The Master's thesis is intended to demonstrate that the student is capable of working independently on an issue in the field of Computational Sciences at an advanced scientific level using scientific methods and to present the findings orally and in writing in an appropriate form, to place them in their scientific context and to document them.
- (2) Students are admitted to the Master's thesis on application if they prove when submitting their application that they
 1. were recently enrolled in the Master's program at the Freie Universität Berlin and
 2. have already successfully completed all the modules in the Synchronization area totaling 30 CP and modules in the Master's program totaling 60 CP or more.
- (3) With the application for admission to the Master's thesis, the students must include proof that the conditions in accordance with paragraph 2 are fulfilled, as well as a statement from an authorized examiner that he/she is willing to supervise the Master's thesis. The relevant examination committee will decide on the application. If a statement of willingness to supervise

the Master's thesis as in clause 1 is not included, the examination committee will appoint a supervisor.

(4) The examination committee sets the topic for the Master's thesis in agreement with the supervisor. Students have the opportunity to make their own suggestions of a topic; the right to take this topic is not guaranteed. The topic and scope of work must be such that they can be completed within the time permitted. Issue of the topic and compliance with the deadline must be recorded.

(5) The Master's thesis is to comprise about 30-80 pages. The time allowed for its completion is 23 weeks. It is to be written in English. If a student is prevented from working on their thesis for longer than three months for a sufficient reason, the examination committee is to decide whether the Master's thesis must be repeated. If the examination committee demands that the Master's thesis be repeated, the examination attainments relating to the Master's thesis are considered invalid.

(6) The Master's thesis is accompanied by a colloquium which usually takes place in the allocated working group. The students are to hold one approx. 30 minute lecture once only on the progress of their Master's thesis.

(7) The date for beginning work on the master's thesis is the date on which the topic was issued by the examination committee. The topic may be returned once within the first four weeks and is considered not to have been issued in this case. When they submit their thesis, students must also confirm in writing that they have written the thesis personally and independently and have used no aids other than the sources and aids listed. Three typed bound copies of the master's thesis and a digital copy in PDF format are to be submitted. The PDF file must contain the text in written form, not in graphic form only and may not be subject to any rights restrictions.

(8) The master's thesis is to be evaluated within four weeks by two authorized examiners appointed by the examination committee and a written statement included. One of the two authorized examiners should be the supervisor of the master's thesis. The examination committee is to ensure that the two people evaluating the thesis represent both the relevant specialization area and the mathematical/computer science principles. If the difference between the grades allocated to the thesis is 2.0 or more, a third evaluation will be commissioned.

(9) The master's thesis gains a 'pass' if the overall grade is at least 'sufficient' (4.0).

Section 10

Retaking examinations

(1) If a student fails the Master's thesis he/she may retake it once. Other program examinations may be retaken three times.

(2) Examinations in the form of a written test given the grade "sufficient" (4.0) may be retaken once to improve the grade in a later examination which is to take place in the first lecture week of the following semester at the latest. The better grade will be taken into account. A repeat examination may not be retaken to improve the grade.

Section 11

Electronic examinations

(1) Electronic examinations take place and are evaluated using digital technologies.

(2) Before an examination using digital technologies takes place, two examiners must check to ensure that the technologies are suitable for the examination tasks and for completing the digital examinations.

(3) The examination candidate's authentic identity and the integrity of the examination results are to be guaranteed. To achieve this, the examination results are to be clearly identified in the form of electronic data and allocated permanently and unmistakably to the student who produced them. It is to be guaranteed that the electronic data for the evaluation and verifiability

are unchanged and complete.

(4) An automatically produced evaluation of an examination is to be checked by an examiner on application by the student examined.

Section 12 Study abroad

(1) Students are recommended to take a period of study abroad. In the course of their studies abroad, students should take courses and examinations (attainments) which can be credited on their Master's program.

(2) Before starting to study abroad, the student should reach an agreement with the chair of the examination board responsible for the program and the relevant authority at the university to be visited, covering the duration of the study period abroad, the attainments to be completed during the study period abroad which must be equivalent to the attainments in the Master's program and the credit points allocated to the attainments. Attainments which comply with the agreement and equivalent attainments will be credited.

(3) Students are recommended to take the period of study abroad during the second or third semester of the Master's program.

Section 13 Final degree

(1) The prerequisite for the award of the final degree is that the attainments required in accordance with Sections 7 and 9 of these regulations have been achieved.

(2) The final degree cannot not awarded if the student has irrevocably failed to achieve the attainment or has irrevocably failed the examination or is in a pending examination procedure at another university in the same program of studies or in a module which is identical to or comparable with a module to be taken in the Master's program and for which the grade is to be included in the overall grade.

(3) The application for confirmation of the final degree must include proof of the fulfilment of the requirements according to paragraph 1 and a statement that none of the cases according to paragraph 2 applies to the applicant. The relevant examination committee will decide on the application.

(4) Students who have passed the examinations are awarded the university degree Master of Science (MSc). The students receive a certificate of academic record and a degree certificate (Annexes 3 and 4) and a diploma supplement (in English and German versions). A further diploma supplement with information on individual modules and their parts (transcript) will also be issued. English versions of the certificate of academic record and degree certificate will also be issued on application.

Section 14 Coming into effect

(1) These regulations come into effect on the day after their publication in the FU Mitteilung [Gazette of the Freie Universität Berlin].

Annex 1: Module descriptions

Explanations:

The following module descriptions specify the following for every module in the Master's program except where other regulations are referred to:

- Module name
- Lecturer responsible for the module
- Admission requirements for each module
- Module content and qualification objectives
- Module teaching and learning units
- Students' estimated workload necessary to complete the module successfully
- Forms of active participation
- Examination forms
- Mandatory regular attendance
- Credit points allocated to each module
- Regular duration of the module
- How often the module is offered
- Applicability of the module

Statements on students' workload required cover the following in particular:

- Active participation in the compulsory attendance phase
- Students' workload required to complete minor tasks in the compulsory attendance phase
- Time for independent preparation and follow-up
- Working on study units in online study phases
- Preparation time for examinations
- Examinations

The notional times given for independent study (including preparation, follow-up and preparation for examinations) are intended as guidance to help the students organize the scheduling of their module-related workload. The statements on workload hours correspond to the number of credit points allocated to the module as a unit of measurement for the student's approximate workload required to complete the module successfully. One credit point is equivalent to 30 hours.

Where attendance is compulsory for the teaching and learning units, it is a prerequisite for the award of the credit points allocated to the module, alongside active participation in the teaching and learning units and successful completion of the module examination. Regular attendance is achieved when the student has attended at least 80% of the teaching and learning units in the module's compulsory attendance phase. If regular attendance at a teaching or learning unit is not compulsory, it is nevertheless strongly recommended. Lecturers may not specify compulsory attendance for learning and teaching units if participation in these is merely recommended in the following.

The module examination must be taken for each module where an examination is scheduled. Graded modules are only complete when the module examination has been taken and passed. The module examination must be related to the module's qualification objectives and is to test that a sample of these aims has been achieved. The examination scope is limited to the amount necessary to do this. In modules where alternative forms of examination are possible, the lecturer responsible for the module must specify the examination form for each semester in the first teaching unit at the latest.

Active participation and – if specified - regular attendance at the module's teaching and learning units and successful completion of the examinations are prerequisites for gaining the credit points allocated to each module.

I. Synchronization area

1. Required modules

| Module: Computational Sciences | | | |
|---|---|---|--|
| University/Department: Freie Universität Berlin/Mathematics and Computer Science | | | |
| Responsible for the module: Module lecturers | | | |
| Admission requirements: none | | | |
| Qualification objectives: The students learn the main interdisciplinary features of scientific work in the computational sciences. They are able to describe problems in the quantitative natural sciences in theoretical terms and to understand the real-world significance of the equations involved. They can formulate the problem in algorithms and identify computer-aided solution methods. They can describe these computer-aided processes numerically and select stable solution methods. They can implement these algorithms, evaluate their time and memory efficiency and optimize them. | | | |
| Content: The main focus of the module is on learning working methods. 1-3 problems of interdisciplinary relevance are selected and scientific theory, algorithmics, numerics and efficiency are rigorously practiced on these examples. In the computer exercises, students work in teams to develop, test and optimize implementations of the problems. Examples of suitable problems are e.g.: <ul style="list-style-type: none"> • <i>Wave phenomena and spectral analysis methods:</i> Waves and oscillations in physics, the Fourier and Laplace transforms, discretization, DFT, FFT, implementation, stability analysis, duration analysis, code optimization, hardware acceleration • <i>Gravitation, electrostatics and computational procedures:</i> gravitation problems and Coulomb's law, periodic systems and convergence, Ewald summation, error analysis, Particle Mesh Ewald, efficient implementation, hardware acceleration • <i>Thermal conductivity equation, Poisson's equation and solution methods:</i> thermal conductivity equation, Poisson's equation, parabolic PDEs, PDEs, analytical solutions for special cases, domain decomposition / finite element approximation, solution using algebraic methods, implementation, convergence analysis, code optimization, hardware acceleration • <i>Data analysis and dimensional reduction:</i> examples of correlated high-dimensional signals, Rayleigh quotient and optimality principle, eigenvalue problem, singular value decomposition and usual solution methods, Nyström approximation and sparse sampling, efficient implementation | | | |
| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) |
| Lecture | 4 | Successful preparation of an efficient commented implementation in teams. Regular presentation of interim findings. Successful completion of project-related tasks. | Lecture contact hours Lecture preparation and follow-up |
| Project seminar | 4 | | PS contact hours PS preparation and follow-up Preparation for examination Examination |
| Module examination | | Written examination (120 minutes) | |
| Module language | | English | |
| Compulsory regular attendance | | Attendance recommended | |
| Workload, total hours | | 450 hours | 15 CP |
| Duration of module | | One semester | |
| Module offered | | Every winter semester | |
| Applicability | | Master's program Computational Sciences | |

2. Discipline-related modules:

a) Chemistry

| |
|---|
| Module: Introduction to Molecular Spectroscopy |
| University/Department: Freie Universität Berlin/Biology, Chemistry, Pharmacy |
| Responsible for the module: Module lecturers |
| Admission requirements: Successful completion of the module Atomic Structure and Chemical Bonding (8 CP) of the Bachelor program Chemistry of the Department of Biology, Chemistry, Pharmacy of the Freie Universität Berlin or equivalent knowledge of quantum mechanics |
| Qualification objectives: The students are able to apply rotational, vibrational, and electronic spectra as important aids in researching geometric structure, electronic structure and energetic and other properties of molecules up to the qualitative analysis of large molecules. Using current examples of optical spectroscopy, the students have gained a deeper knowledge of the relationships and understand the fundamental significance of spectroscopy in science and technology. They solve practice problems and discuss their solutions in groups. |
| Content: Physical principles of electromagnetic radiation, interaction of electromagnetic radiation with material with /without absorption and emissions of photons, experimental aspects, rotational spectroscopy, vibrational spectroscopy, electronic transitions |

| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) | |
|-------------------------------------|---|---|---|----------------|
| Lecture | 2 | - | Lecture contact hours Lecture preparation and follow-up | 30 30 |
| Practice seminar | 2 | Work on practice tasks, contributions to discussion | Prac.S contact hours Prac.S preparation and follow-up Preparation for examination | 30 30 30 |
| Module examination | | Written examination (120 Minutes) or oral examination (approx. 30 Minutes) or term paper (approx. 15 pages); the module examination is not evaluated in detail. | | |
| Module language | | German | | |
| Mandatory regular attendance | | Attendance recommended | | |
| Workload, total hours | | 150 hours | 5 CP | |
| Duration of module | | One semester | | |
| Module offered | | At least once per academic year | | |
| Applicability | | Master's program Computational Sciences | | |

| Module: Introduction to Theoretical Chemistry | | | | |
|--|---|--|--|----------------------|
| University/Department: Freie Universität Berlin/Biology, Chemistry, Pharmacy | | | | |
| Responsible for the module: Module lecturers | | | | |
| Admission requirements: none | | | | |
| Qualification objectives: The students are familiar with fundamental analytical and numerical concepts and methods of theoretical chemistry. They can apply time-independent and time-dependent quantum mechanical methods for selected model systems in chemistry and have the numerical skills to carry out the appropriate computer simulations. This gives them a deeper understanding of the properties of molecules and chemical reactions. | | | | |
| Content: In-depth mathematical representation of time-independent and time-dependent quantum mechanics, solving quantum mechanical one-particle problems (free particle, harmonic oscillator, hydrogen atom), dynamics of the nucleus (oscillation and rotation), nucleus oscillations of multi-atom molecules, time-dependent and time-independent calculation of perturbations, selected numerical solution methods for calculating time-dependent quantum mechanical model systems | | | | |
| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) | |
| Lecture | 2 | - | Lecture contact hours Lecture preparation and follow-up | 30 30 |
| Practice seminar | 1 | Contributions to discussion, Presentation of selected simulation findings | Prac.S contact hours Supervised computer exercise Independent computer work Prac.S preparation and follow-up Preparation for examination | 15 15 30 30 |
| Module examination | | Practical examination (approx. 30 minutes); the module examination is not evaluated in detail. | | |
| Module language | | German | | |
| Mandatory regular attendance | | Attendance recommended | | |
| Workload, total hours | | 150 hours | 5 CP | |
| Duration of module | | One semester | | |
| Module offered | | Every winter semester | | |
| Applicability | | Master's program Computational Science | | |

| | | | | |
|--|--|--|--|--|
| Module: Quantum Mechanical Description of Atoms and Chemical Bonding | | | | |
| University/Department: Freie Universität Berlin/Biology, Chemistry, Pharmacy | | | | |
| Responsible for the module: Module lecturers | | | | |
| Admission requirements: none | | | | |
| Qualification objectives: The students have a basic understanding of quantum mechanics and its application to simple chemically relevant examples. They can use mathematical tools to describe the electron structures of atoms and small molecules and are familiar with atomic models and the quantum mechanical principles of spectroscopic measurement. | | | | |

| They know the connections of quantum theory with orbitals and chemical bonding. They can analytically examine simple issues on the quantum nature of chemical model systems independently and in groups using selected numerical methods, prepare them for teaching purposes and present them appropriately in gender-specific and diversity-specific ways. | | | | |
|--|---|--|--|--------------------|
| Content: Introduction to the quantum nature of matter and energy, principles of quantum theory, quantum mechanical solutions of the time-independent Schrödinger equation for chemically relevant model systems, quantum theory of orbital angular momentum and spin. Quantum mechanics of the hydrogen atom, multi-electron atoms, spin-orbit coupling, theory of chemical bonding, elementary quantum theory of simple molecules. Analytical and numerical solution methods for simple quantum mechanical problems. | | | | |
| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) | |
| Lecture | 4 | - | Lecture contact hours Lecture preparation and follow-up | 60 70 |
| Practice seminar | 2 | Work on practice tasks, Contributions to discussion Developing and presenting a quantum theoretical topic using numerical methods | Prac.S contact hours Prac.S preparation and follow-up Preparation for examination Examination | 30 70 70 |
| Module examination | | Written examination (180 minutes), which may also be carried out as an electronic examination, or oral examination (approx. 30 minutes) or term paper (approx. 15 pages); the module examination is not evaluated in detail. | | |
| Module language | | German | | |
| Compulsory regular attendance | | Attendance recommended | | |
| Workload, total hours | | 300 hours | | 10 CP |
| Duration of module | | One semester | | |
| Module offered | | Every semester | | |
| Applicability | | Master's program Computational Sciences | | |

b) Geographical sciences

| Module: Principles of Remote Sensing and Digital Image Analysis | | | | |
|---|---|---|--|--------------------|
| University/Department: Freie Universität Berlin/Earth Sciences | | | | |
| Responsible for the module: Module lecturers | | | | |
| Admission requirements: none | | | | |
| Qualification objectives: The students have basic skills and competences in digital remote sensing and digital image analysis in the earth sciences. They can work independently and in groups to examine issues in remote sensing and image analysis, using selected numerical methods, prepare the issues didactically and present them in a gender-specific and diversity-specific way. | | | | |
| Content: The module gives a theoretical introduction to the topic; selected aspects are studied in more detail and practiced in relation to practical examples, using current software packages. The topics include the principles of: <ul style="list-style-type: none"> - Introduction to radiation physics - Principles of photogrammetry - Digital and analog passive image recording systems - Visualization of multispectral data - Principles of image analysis - Special image extraction (e.g. indices, PCA) - Interpretation of remote sensing data - Time series analysis with raster data (change detection) - Multispectral classification method - Introduction to active remote sensing systems | | | | |
| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) | |
| Lecture | 2 | - | Lecture contact hours Lecture preparation and follow-up | 30 20 |
| Seminar | 2 | Practice tasks | Contact hours S Preparation and follow-up S Preparation for examination Examination | 30 25 45 |
| Module examination | | Written examination (90 minutes), which may also be carried out as an electronic examination, or oral examination (approx. 30 minutes) or term paper (approx. 15 pages); the module examination is not evaluated in detail. | | |
| Module language | | German | | |

| | | |
|-------------------------------------|--|------|
| Mandatory regular attendance | Attendance recommended | |
| Workload, total hours | 150 hours | 5 CP |
| Duration of module | One semester | |
| Module offered | At least once per academic year, every winter semester | |
| Applicability | Master's program Computational Sciences | |

Module: Principles of Hydrogeography and Climate Geography
University/Department: Freie Universität Berlin/Earth Sciences

Responsible for the module: Module lecturers

Admission requirements: none

Qualification objectives: The students have mastered fundamental knowledge on climate geography and hydrogeography, in particular the specialist terminology, and can apply it in scientific discourse. They can describe global relationships of the climate system including the interaction with the oceans, the general circulation of the atmosphere and elements of the water cycle.

Content: The module presents the principles of climate geography and hydrogeography. This includes among other things the principles of the climate system; the radiation budget and thermal budget; general circulation of the atmosphere; climate classifications; role of the oceans in the climate system; elements of the water cycle and their space-time characteristics and metrological determination; water balance and water budget on various levels of scale. Students study selected content in more detail, working on practice tasks independently or in small groups. In addition, the module gives an introduction to scientific work, in particular using specialist literature, e.g. principles of literature preparation and correct references to scientific texts.

| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) | |
|--------------------------------------|--|---|--|--------------------|
| Lecture | 2 | - | Lecture contact hours Lecture preparation and follow-up | 30 15 |
| Seminar | 2 | Practice tasks, presentation | S contact hours S preparation and follow-up Preparation for examination Examination | 30 30 45 |
| Module examination | | Written examination (90 minutes), which may also be carried out as an electronic examination, or oral examination (approx. 30 minutes) or term paper (approx. 15 pages); the module examination is not evaluated in detail. | | |
| Module language | German | | | |
| Compulsory regular attendance | Attendance recommended | | | |
| Workload, total hours | 150 hours | | | 5 CP |
| Duration of module | Two semesters | | | |
| Module offered | At least once per academic year, every winter semester | | | |
| Applicability | Master's program Computational Sciences | | | |

Module: Principles of Geographical Information Systems

University/Department: Freie Universität Berlin/ Earth Sciences

Responsible for the module: Module lecturers

Admission requirements: none

Qualification objectives: The students have gained the fundamental skills and competences of digital spatial information processing for work in earth sciences. They can examine issues relating to geographical information systems independently and in groups, using selected computer-aided methods, prepare them for teaching purposes and present them in a gender-specific and diversity-specific way.

Content: The module gives a theoretical introduction to the topic. Selected aspects are studied in more detail and practiced in relation to practical examples, using current software packages. It covers the principles of:

- Structure and applications of geoinformation systems
- Data models (raster data /vector data)
- Methods and problems of imaging geospace (geodetic reference systems)
- Georeferencing
- Extracting and processing vector data
- Processing spatial and attributive information
- Geodatabases
- Interpolation methods
- Preparing and analyzing digital terrain models
- Extracting hydrological parameters
- Visualizing geodata
- Interfaces of geodata processing
- Developing and preparing maps
- Principles of remote sensing

| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) |
|-----------------------------|---|-------------------------------|---------------------|
|-----------------------------|---|-------------------------------|---------------------|

| | | | | |
|--------------------------------------|---|---|--|--------------------|
| Lecture | 2 | - | Lecture contact hours Lecture preparation and follow-up | 30 20 |
| Seminar | 2 | Practice tasks | S contact hours S preparation and follow-up Preparation for examination Examination | 30 25 45 |
| Module examination | | Written examination (90 minutes), which may also be carried out as an electronic examination, or oral examination (approx. 30 minutes) or term paper (approx. 15 pages); the module examination is not evaluated in detail. | | |
| Module language | | German | | |
| Compulsory regular attendance | | Attendance recommended | | |
| Workload, total hours | | 150 hours | | 5 CP |
| Duration of module | | One semester | | |
| Module offered | | At least once per academic year every summer semester | | |
| Applicability | | Master's program Computational Sciences | | |

c) Geological Sciences

| Module: Synchronization Earth | | | | |
|---|---|---|--|--------------------|
| University/Department: Freie Universität Berlin/Earth Sciences | | | | |
| Responsible for the module: Module lecturers | | | | |
| Admission requirements: none | | | | |
| Qualification objectives: The students gain a thorough understanding of the structure, composition and process of our planet and the earth's uniqueness in comparison to other planets. They gain an insight into the physical and chemical processes which shape the surface and the driving forces behind them in the earth's interior. They know the earth's structure and its significance and have learnt the methods used by earth scientists to examine the earth's interior. The students are familiar with geological cycles and their time frames. They are able to identify the most important rock-forming minerals and rocks and can classify them according to their formation conditions. The students have an advanced understanding of our planet's structure, composition and processes. They understand the principles of the interaction between the earth's solid structure, the atmosphere, the hydrosphere and biosphere and of (mostly exogenic) processes in different time scales. | | | | |
| Content: The module covers the following topics: fundamental systems and processes of planet earth; space and time; material components; geoscientific cycles; interaction between hydrosphere, atmosphere, geosphere; relative and absolute age; sedimentary cycles (weathering, erosion, sedimentation); phenomenological geophysics; magmatism; metamorphism; structure; plate tectonics; processes and mutual interaction of tectonics, weathering, erosion, climate, transport processes and depositional environments depending on exogenic and endogenic variables; influence of organisms on these processes; carbon cycle; climate change; surface-shaping processes in the interplay of climate, atmospheric composition and tectonics; mass balances and flow behaviors in global systems. The students study the macroscopic identification of minerals and rocks. | | | | |
| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) | |
| Introductory course 1 | 2 | - | IC 1 contact hours IC 1 preparation and follow-up | 30 45 |
| Practical | 2 | Successful completion of practice tasks | P contact hours P preparation and follow-up | 30 60 |
| Introductory course 2 | 2 | - | IC2 contact hours IC2 preparation and follow-up Preparation for examination Examination | 30 45 60 |
| Module examination | | Written examination (90 minutes), which may also be carried out as an electronic examination, or oral examination (approx. 30 minutes) or term paper (approx. 15 pages); the module examination is not evaluated in detail. | | |
| Module language | | German | | |
| Compulsory regular attendance | | Attendance recommended | | |
| Workload, total hours | | 300 hours | | 10 CP |
| Duration of module | | Two semesters | | |
| Module offered | | At least once per academic year (IC1 und P in the winter semester, IC2 in the summer semester) | | |
| Applicability | | Master's program Computational Sciences | | |

d) Computer Science

| Module: Complex Algorithms A | | | | |
|--|---|---|-----------------------------------|-------|
| University/Department: Freie Universität Berlin/Mathematics and Computer Science | | | | |
| Responsible for the module: Module lecturers | | | | |
| Admission requirements: none | | | | |
| Qualification objectives: The students have mastered the principles of the current design techniques for algorithms and can use them to design algorithms. They can analyze algorithms in relation to their time and memory requirements, applying advanced analytical methods. They understand the principles of the theory of NP completeness. They know the most common complexity classes and can classify simple problems according to their complexity. They further develop these skills independently in a selected topic area of higher computer science. The students can apply complex algorithms to one of the following topics: distributed systems, pattern recognition, database technology or artificial intelligence. | | | | |
| Content: The module covers aspects of the following topics: path and flow problems in graphs; string matching; randomized algorithms; amortized analysis; the 'master theorem' for the analysis of divide-and-conquer recursion equations; NP completeness; approximation algorithms for difficult problems; number-theoretic algorithms (including RSA cryptosystems); arithmetic algorithms and circuits and Fast Fourier Transform. These topics are subsequently examined in more depth, using examples. The following topics are offered: | | | | |
| <ul style="list-style-type: none"> - Distributed systems, distributed algorithms, distributed data management, search methods for solving combinatorial tasks - First-order logic and its mechanization, resolution and theorem proofs, knowledge-based and expert systems, fuzzy logic - Bayesian pattern recognition, clustering, expectation maximization, neural networks and learning algorithms, associative networks, recurrent networks. Computer vision with neural networks - Database access technologies and query optimization; realization of transactions, particularly synchronization methods; technological measures to make database systems fault-tolerant. Methods of efficient management of different types of large data sets, in particular of XML documents; correct implementation of transactional guarantees in data management systems | | | | |
| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) | |
| Lecture | 4 | - | Lecture contact hours | 60 |
| | | | Lecture preparation and follow-up | 80 |
| Practice seminar | 2 | - written completion of the work sheets - two oral presentations, each showing the solution of one practice task in the practice seminar | S contact hours | 30 |
| | | | S preparation and follow-up | 60 |
| | | | Prac.S contact hours | 30 |
| | | | Prac.S preparation and follow-up | 60 |
| Seminar | 2 | Preparation and presentation of a research topic | Written practice tasks | 70 |
| | | | Preparation for examination | |
| | | | Examination | |
| Module examination | | Written examination (90 minutes), which may also be carried out as an electronic examination, or oral examination (approx. 30 minutes) or term paper (approx. 15 pages); the module examination is not evaluated in detail. | | |
| Module language | | German | | |
| Compulsory regular attendance | | Attendance recommended | | |
| Workload, total hours | | 450 hours | | 15 CP |
| Duration of module | | One or two semesters | | |
| Module offered | | At least once per academic year | | |
| Applicability | | Master's program Computational Sciences | | |

| | | | | |
|---|--|--|--|--|
| Module: Computer Science and Data Structures A | | | | |
| University/Department: Freie Universität Berlin/Mathematics and Computer Science | | | | |
| Responsible for the module: Module lecturers | | | | |
| Admission requirements: none | | | | |
| Qualification objectives: The students possess basic skills in developing object-oriented software: they can deal with data abstraction, inheritance, and polymorphic type systems and are able to specify and implement abstract data types, to carry out soundness proofs for the implementation of abstract data types, and to take decisions on selecting the data representation method in each case, taking efficiency analyses into account. They are familiar with the main abstract data types and their current implementations and the relevant interfaces and classes from the libraries of the programming language used. | | | | |
| Content: The module's starting point is information hiding and its significance for structuring programs and constructing data objects using modules and classes. The term data abstraction, linked with the distinction between specification and implementation of abstract data objects and data types, plays a crucial part in data modeling. Sequences, sets, relations, trees, graphs and geometrical objects are introduced as abstract types. Finally, efficiently manipulable | | | | |

representations of these types are studied and the complexity of the related algorithms examined.

| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) | |
|--------------------------------------|---|---|-----------------------------------|-------|
| Lecture | 4 | - | Lecture contact hours | 60 |
| | | | Lecture preparation and follow-up | 80 |
| Practice seminar | 2 | - written completion of the work sheets - two oral presentations, each showing the solution of one practice task in the practice seminar | S contact hours | 30 |
| | | | S preparation and follow-up | 60 |
| | | | Prac.S contact hours | 30 |
| | | | Prac.S preparation and follow-up | 60 |
| Seminar | 2 | Preparation and presentation of a programming project | Written practice tasks | 70 |
| | | | Preparation for examination | |
| | | | Examination | |
| Module examination | | Written examination (90 minutes), which may also be carried out as an electronic examination, or oral examination (approx. 30 minutes) or term paper (approx. 15 pages); the module examination is not evaluated in detail. | | |
| Module language | | German | | |
| Compulsory regular attendance | | Attendance recommended | | |
| Workload, total hours | | 450 hours | | 15 CP |
| Duration of module | | One or two semesters | | |
| Module offered | | At least once per academic year | | |
| Applicability | | Master's program Computational Sciences | | |

Module: Computer Science and Functional Programming A

University/Department: Freie Universität Berlin/Mathematics and Computer Science

Responsible for the module: Module lecturers

Admission requirements: none

Qualification objectives: The students are able to functionally design elementary algorithms, to formally specify demands on functional programs, to develop well-structured functional programs, to examine the complexity of functional programs and to formally prove the properties of functional programs. They understand the principles of computability.

Content: Principles of computability (Lambda calculus, primitive recursion, μ -recursion). Introduction to functional programming (syntax, primitive data types, lists, tuples, strings, expressions, function definitions, recursion and iteration, higher order functions, polymorphism, type systems, type inference and type checking, algebraic and abstract data types, input and output, search and sorting algorithms). Proofs of program properties (rewriting, structural induction, scheduling). Implementation and programming technique (evaluation strategies for functional programs, modular program design)

| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) | |
|--------------------------------------|---|---|-----------------------------------|-------|
| Lecture | 4 | - | Lecture contact hours | 60 |
| | | | Lecture preparation and follow-up | 80 |
| Practice seminar | 2 | - written completion of the work sheets - two oral presentations, each showing the solution of one practice task in the practice seminar | S contact hours | 30 |
| | | | S preparation and follow-up | 60 |
| | | | Prac.S contact hours | 30 |
| | | | Prac.S preparation and follow-up | 60 |
| | | | Written practice tasks | 60 |
| Seminar | 2 | Preparation and presentation of a programming project | | 70 |
| | | | Preparation for examination | |
| | | | Examination | |
| Module examination | | Written examination (90 minutes), which may also be carried out as an electronic examination, or oral examination (approx. 30 minutes) or term paper (approx. 15 pages); the module examination is not evaluated in detail. | | |
| Module language | | German | | |
| Compulsory regular attendance | | Attendance recommended | | |
| Workload, total hours | | 450 hours | | 15 CP |
| Duration of module | | One or two semesters | | |
| Module offered | | At least once per academic year | | |
| Applicability | | Master's program Computational Sciences | | |

| Module: Computer Science and Object-Oriented Programming A | | | |
|---|---|---|--|
| University/Department: Freie Universität Berlin/Mathematics and Computer Science | | | |
| Responsible for the module: Module lecturers | | | |
| Admission requirements: none | | | |
| Qualification objectives: The students can specify algorithms in relation to their condition, develop well-structured imperative programs, analyze the complexity of imperative programs and formally prove the properties of imperative programs. | | | |
| Content: Principles of computability (universal register machines, syntax and operational semantics of imperative programming languages); formal methods for specification and verification of imperative programs: (conditions of the state-space, Hoare logic, partial soundness, termination); concepts of imperative and object-oriented programming (primitive and combined data types, methods, parameter passing, overloading, modules, classes, objects, class hierarchies, inheritance, abstract classes, interfaces); programming methodology (incremental correct program development, divide-and-conquer, backtracking, analysis of time and memory requirements, big O notation, transformation of recursion into iteration, analysis of search and sorting algorithms) | | | |
| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) |
| Lecture | 4 | - | Lecture contact hours 60 Lecture preparation and follow-up 80 |
| Practice seminar | 2 | - written completion of the work sheets - two oral presentations, each showing the solution of one practice task in the practice seminar | S contact hours 30 S preparation and follow-up 60 Prac.S contact hours 30 Prac.S preparation and follow-up 60 |
| Seminar | 2 | Preparation and presentation of a programming project | Written practice tasks 70 Preparation for examination Examination |
| Module examination | | Written examination (90 minutes), which may also be carried out as an electronic examination, or oral examination (approx. 30 minutes) or term paper (approx. 15 pages); the module examination is not evaluated in detail. | |
| Module language | | German | |
| Compulsory regular attendance | | Attendance recommended | |
| Workload, total hours | | 450 hours | 15 CP |
| Duration of module | | one or two semesters | |
| Module offered | | At least once per academic year | |
| Applicability | | Master's program Computational Sciences | |

e) Mathematics

| Module: Introduction to Numerical Mathematics A | | | |
|--|---|---|---|
| University/Department: Freie Universität Berlin/Mathematics and Computer Science | | | |
| Responsible for the module: Module lecturers | | | |
| Admission requirements: none | | | |
| Qualification objectives: The students have mastered basic numerical solution methods for elementary algebra problems and ordinary differential equations. They have developed a sense for the mathematical structure of these problems and can select and develop reliable and efficient solution algorithms. During the seminars, the students have applied what they have learnt to practical problems of scientific computation and gained an insight into the mathematical modeling of this type of problem. | | | |
| Content: Solution methods for linear equation systems; Cholesky decomposition and QR decomposition; eigenvalue problems; best approximations; polynomial and spline interpolation; Gaussian quadrature and adaptive quadrature; initial value problems for ordinary differential equations | | | |
| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) |
| Lecture | 4 | - | Lecture contact hours 60 Lecture preparation and follow-up 80 |
| Practice seminar | 2 | Successful completion of practice tasks | S contact hours 30 S preparation and follow-up 60 |
| Seminar | 2 | Preparation and presentation of a research topic or programming project | Prac.S contact hours 30 Prac.S preparation and follow-up 60 Written practice tasks 70 |

| | | | |
|--------------------------------------|---|--|---|
| | | | Preparation for examination Examination |
| Module examination | Written examination (90 minutes), which may also be carried out as an electronic examination, or oral examination (approx. 30 minutes) or term paper (approx. 15 pages); the module examination is not evaluated in detail. | | |
| Module language | German | | |
| Compulsory regular attendance | Attendance recommended | | |
| Workload, total hours | 450 hours | | 15 CP |
| Duration of module | One or two semesters | | |
| Module offered | At least once per academic year | | |
| Applicability | Master's program Computational Sciences | | |

| Module: Numerics of ODEs and numerical linear algebra A | | | |
|---|---|---|--|
| University/Department: Freie Universität Berlin/Mathematics and Computer Science | | | |
| Responsible for the module: Module lecturers | | | |
| Admission requirements: none | | | |
| Qualification objectives: The students have mastered basic numerical solution methods for ordinary differential equations and have a basic knowledge of numerical linear algebra and can deal these topics confidently. During the seminars, the students have applied what they have learnt to practical problems of scientific computation and gained an insight into the mathematical modeling of this type of problem. | | | |
| Content: Selection from the following topics: - Initial value problems for stiff differential equations (stability and asymptotic stability of fixed points, test equations) - implicit Runge-Kutta methods (inheritance methods, stability fields, A- and B-stability, Gaussian method) - differential algebraic equations (basic terminology, index) - Hamiltonian systems (energy conservation, symplecticism, symplectic Rung-Kutta method) - Iterative methods for solving large linear equation systems (linear iterative method, preconditioning, method of steepest descent, conjugate gradient method) | | | |
| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) |
| Lecture | 4 | - | Lecture contact hours 60 Lecture preparation and follow-up 80 |
| Practice seminar | 2 | Successful completion of practice tasks | S contact hours 30 S preparation and follow-up 60 |
| Seminar | 2 | Preparation and presentation of a research topic or programming project | Prac.S contact hours 60 Prac.S preparation and follow-up 60 Written practice tasks 70 Preparation for examination Examination |
| Module examination | Written examination (90 minutes), which may also be carried out as an electronic examination, or oral examination (approx. 30 minutes) or term paper (approx. 15 pages); the module examination is not evaluated in detail. | | |
| Module language | German or English | | |
| Compulsory regular attendance | Attendance recommended | | |
| Workload, total hours | 450 hours | | 15 CP |
| Duration of module | One or two semesters | | |
| Module offered | At least once per academic year | | |
| Applicability | Master's program Computational Sciences | | |

| | | | |
|---|--|--|--|
| Module: Numerics of partial differential equations A | | | |
| University/Department: Freie Universität Berlin/Mathematics and Computer Science | | | |
| Responsible for the module: Module lecturers | | | |
| Admission requirements: none | | | |
| Qualification objectives: The students have gained a fundamental knowledge of numerical solutions for partial differential equations and numerical linear algebra and can deal with them confidently. During the seminars, the students have applied what they have learnt to practical problems of scientific computation and gained an insight into the mathematical modeling of this type of problem. | | | |
| Content: Selection from the following topics: - Mathematical modeling with partial differential equations - Classification (elliptic, parabolic, hyperbolic) and well-posedness - Classical solutions and finite differences (maximum principle, consistency, convergence) - Weak solutions and finite elements (Sobolev spaces, error estimates, partial volume correction methods) - Parabolic differential equations (method of lines, Rothe's method) | | | |

| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) | |
|--------------------------------------|---|---|-----------------------------------|-------|
| Lecture | 4 | - | Lecture contact hours | 60 |
| | | | Lecture preparation and follow-up | 80 |
| Practice seminar | 2 | Successful completion of practice tasks | S contact hours | 30 |
| | | | S preparation and follow-up | 60 |
| Seminar | 2 | Preparation and presentation of a research topic or programming project | Prac.S contact hours | 30 |
| | | | Prac.S preparation and follow-up | 60 |
| | | | Written practice tasks | 70 |
| | | | Preparation for examination | |
| | | | Examination | |
| Module examination | | Written examination (90 minutes), which may also be carried out as an electronic examination, or oral examination (approx. 30 minutes) or term paper (approx. 15 pages); the module examination is not evaluated in detail. | | |
| Module language | | German or English | | |
| Compulsory regular attendance | | Attendance recommended | | |
| Workload, total hours | | 450 hours | | 15 CP |
| Duration of module | | One or two semesters | | |
| Module offered | | At least once per academic year | | |
| Applicability | | Master's program Computational Sciences | | |

Module: Synchronization Mathematics

University/Department: Freie Universität Berlin/Physics, Mathematics and Computer Science

Responsible for the module: Module lecturers

Admission requirements: none

Qualification objectives: The students have gained an overview of the structure and aims of mathematics and their working methods. They also have a grasp of the core structures and clause-sets of linear algebra and of computation with matrices and vectors. They can map algebraic problems on the computer and solve them using numerical methods.

Content:

- *Linear algebra:* Working methods and aims of mathematics, logic, sets and maps, algebraic structures, fields, real numbers, complex numbers, linear maps, linear equation systems, matrices, representations and changes of basis, determinants, eigenvalues and eigenvectors, scalar products, orthogonal systems
- *Computer-oriented mathematics:* Using computers to solve mathematical problems. Number description, round-off errors, condition, stability, complexity and efficiency
- *Computer algebra systems:* Principles of use and script-based programming

| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) | |
|--------------------------------------|---|--|-----------------------------------|-------|
| Lecture | 4 | - | Lecture contact hours | 90 |
| | | | Lecture preparation and follow-up | 150 |
| Practice seminar | 2 | Successful completion of practice tasks | | 60 |
| Lecture | 2 | - | Prac.S contact hours | 60 |
| | | | Prac.S preparation and follow-up | 60 |
| | | | Written practice tasks | |
| Practice seminar | 2 | Successful completion of practice tasks | Preparation for examination | 30 |
| | | | Examination | |
| Module examination | | Written examination (90 minutes) or oral examination (approx. 30 minutes) or term paper (approx. 15 pages); the module examination is not evaluated in detail. | | |
| Module language | | German | | |
| Compulsory regular attendance | | Attendance recommended | | |
| Workload, total hours | | 450 hours | | 15 CP |
| Duration of module | | One or two semesters | | |
| Module offered | | At least once per academic year | | |
| Applicability | | Master's program Computational Sciences | | |

f) Meteorology

Module: Atmospheric Dynamics

University/Department: Freie Universität Berlin/Earth Sciences

Responsible for the module: Module lecturers

| Admission requirements: none | | | |
|---|---|---|--|
| Qualification objectives: The students have a grasp of hydrodynamics and thermodynamics specific to the specialization area Atmospheric Sciences, which form the theoretical basis for practical weather prediction in the synoptic scale area. They can understand in physical terms the most important formation mechanisms of mid-latitude high-pressure and low-pressure areas and can analyze them independently. | | | |
| Content: The module covers topics such as introduction to derived values of divergence, vorticity and deformation; comprehensive evaluation of the basic equations for gaining meteorological statements on the synoptic scale with the aid of derived values; discussion of the quasi-geostrophic baroclinic model of the atmosphere; introduction to basic large-scale vorticity and the concept of potential vorticity; land-sea wind circulation; planetary waves and the main instability processes in the atmosphere; theory of general atmospheric circulation. | | | |
| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) |
| Lecture | 4 | - | Lecture contact hours 60 Lecture preparation and follow-up 50 |
| Practice seminar | 2 | Successful completion of practice tasks | Prac.S contact hours 30 Prac.S preparation and follow-up 50 Preparation for Examination 50 |
| Module examination | | Written examination (90 minutes), which may also be carried out as an electronic examination, or oral examination (approx. 30 minutes) or term paper (approx. 15 pages); the module examination is not evaluated in detail. | |
| Module language | | German | |
| Compulsory regular attendance | | Attendance recommended | |
| Workload, total hours | | 240 hours | 8 CP |
| Duration of module | | One semester | |
| Module offered | | At least once per academic year | |
| Applicability | | Master's program Computational Sciences | |

| Module: Introduction to Atmospheric Dynamics | | | |
|---|---|---|---|
| University/Department: Freie Universität Berlin/Earth Sciences | | | |
| Responsible for the module: Module lecturers | | | |
| Admission requirements: none | | | |
| Qualification objectives: The students have a grasp of applied hydrodynamics and thermodynamics in meteorology. They are familiar with the basic meteorological equation system and can apply the terminology of the scales, conserved quantities and wind approximation in the meteorological context. | | | |
| Content: The module covers topics such as atmospheric thermodynamics; changes to atmospheric air conditions; atmospheric structure; polytropic atmospheres; water vapor and latent heat; principles of kinematics; derivation of the prognostic basic meteorological equations from classical hydrodynamics and thermodynamics; scale terminology in meteorology; Lagrangian and Eulerian representations; natural coordinates; basic balances (geostrophic wind, cyclostrophic wind, gradient wind) and thermal wind. | | | |
| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) |
| Lecture | 4 | Successful completion of practice tasks | Lecture contact hours 60 Lecture preparation and follow-up 150 |
| Module examination | | none | |
| Module language | | German | |
| Compulsory regular attendance | | Attendance recommended | |
| Workload, total hours | | 210 hours | 7 CP |
| Duration of module | | One semester | |
| Module offered | | At least once per academic year | |
| Applicability | | Master's program Computational Sciences | |

| | | | |
|---|--|--|--|
| Module: Principles of Synoptic Meteorology | | | |
| University/Department: Freie Universität Berlin/Earth Sciences | | | |
| Responsible for the module: Module lecturers | | | |
| Admission requirements: none | | | |
| Qualification objectives: The students understand the three-dimensional spatial and temporal structures, processes and interactions that determine the weather conditions on the synoptic, global and convective scales in the mid-latitudes. They can analyze, classify, present and evaluate the current weather situation on the basis of weather maps. | | | |
| Content: The module covers topics such as the introduction of three-dimensional diagnosis of mid-latitude synoptic-scale weather systems: air masses and fronts, cyclones and anti-cyclones, jet streams and waves of the west wind zone, their temporal development and relation to weather phenomena. Practical work on the DWD's (graphic) system Niño is introduced and carried out independently. This includes analyzing current global examples related to the content of each lecture. Solving practical tasks helps the students to develop a basic understanding of the lecture content. | | | |

Analysis and discussion of the current weather situation in the European-Atlantic sector by means of meteorological fields and satellite images.

| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) | |
|--------------------------------------|---|--|-----------------------------------|----|
| Lecture | 2 | - | Lecture contact hours | 30 |
| | | | Lecture preparation and follow-up | 65 |
| Practice seminar | 2 | Successful completion of practice tasks, lecture | Prac.S contact hours | 30 |
| | | | Prac.S preparation and follow-up | 85 |
| Module examination | | none | | |
| Module language | | German | | |
| Compulsory regular attendance | | Attendance recommended | | |
| Workload, total hours | | 210 hours | 7 CP | |
| Duration of module | | One semester | | |
| Module offered | | At least once per academic year | | |
| Applicability | | Master's program Computational Sciences | | |

g) Physics

| Module: Computational Statistical Physics I A | | | | |
|---|---|---|-----------------------------------|----|
| University/Department: Freie Universität Berlin/Physics | | | | |
| Responsible for the module: Module lecturers | | | | |
| Admission requirements: none | | | | |
| Qualification objectives: The students are able to name and describe the principle concepts and theorems of statistical physics and thermodynamics. They are also capable of applying the methods they have learnt to given problems and to solve them. The students have also mastered the computation methods necessary for dealing with statistical physics and thermodynamics and are able to apply them. They can apply their knowledge of methodology and computation methods in the field of statistical physics to complex issues. | | | | |
| Content: Elementary statistics and the laws of large numbers, equilibrium ensembles, the principle of maximum entropy, main theorems of thermodynamics, thermodynamic potentials, thermodynamic processes, phase transition, ideal quantum gases, interactive systems. | | | | |
| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) | |
| Lecture | 4 | - | Lecture contact hours | 60 |
| | | | Lecture preparation and follow-up | 80 |
| Practice seminar | 2 | Successful completion of practice tasks | S contact hours | 30 |
| | | | S preparation and follow-up | 60 |
| Seminar | 2 | Preparation and presentation of a research topic or programming project | Prac.S contact hours | 30 |
| | | | Prac.S preparation and follow-up | 60 |
| | | | Written practice tasks | 70 |
| Module examination | | Written examination (90 minutes), which may also be carried out as an electronic examination, or oral examination (approx. 30 minutes) or term paper (approx. 15 pages); the module examination is not evaluated in detail. | | |
| Module language | | English | | |
| Compulsory regular attendance | | Attendance recommended | | |
| Workload, total hours | | 450 hours | 15 CP | |
| Duration of module | | One or two semesters | | |
| Module offered | | At least once per academic year | | |
| Applicability | | Master's program Computational Sciences | | |

| | | | | |
|---|--|--|--|--|
| Module: Computational Statistical Physics II A | | | | |
| University/Department: Freie Universität Berlin/Physics | | | | |
| Responsible for the module: Module lecturers | | | | |
| Admission requirements: none | | | | |
| Qualification objectives: The students have a grasp of the fundamental concepts and theorems of statistical physics. They can name, describe and apply them and apply the methods they have learnt to existing problems to solve them. The students have extended their knowledge of methods and calculation methods in the field of statistical physics and are now able to apply these to complex issues. Using the methods they have learnt, they are also able to derive and analyze microscopic physical processes / laws at the macroscopic level. | | | | |
| Content: A selection of the following advanced topics of statistical physics: non-equilibrium thermodynamics (entropy production, Onsager relations), linear response theory and fluctuation-dissipation theorem, stochastic processes | | | | |

(Markov processes, master equation, Langevin equation and Fokker-Planck equation), kinetic theory, phase transition (Landau theory, Gaussian fluctuations, correlation functions, renormalization groups), theory of liquids, hydrodynamics and elasticity, statistical quantum mechanics, exactly solvable models.

| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) | |
|--------------------------------------|---|---|-----------------------------------|-------|
| Lecture | 4 | - | Lecture contact hours | 60 |
| | | | Lecture preparation and follow-up | 80 |
| Practice seminar | 2 | Successful completion of practice tasks | S contact hours | 30 |
| | | | S preparation and follow-up | 60 |
| Seminar | 2 | Preparation and presentation of a research topic or programming project | Prac.S contact hours | 30 |
| | | | Prac.S preparation and follow-up | 60 |
| | | | Written practice tasks | 70 |
| | | | Preparation for examination | |
| | | | Examination | |
| Module examination | Written examination (90 minutes), which may also be carried out as an electronic examination, or oral examination (approx. 30 minutes) or term paper (approx. 15 pages); the module examination is not evaluated in detail. | | | |
| Module language | English | | | |
| Compulsory regular attendance | Attendance recommended | | | |
| Workload, total hours | 450 hours | | | 15 CP |
| Duration of module | One or two semesters | | | |
| Module offered | At least once per academic year | | | |
| Applicability | Master's program Computational Sciences | | | |

Module: Introduction to Quantum Mechanics

University/Department: Freie Universität Berlin/Physics

Responsible for the module: Module lecturers

Admission requirements: none

Qualification objectives: The students learn the basic mathematical and methodological concepts of the quantum mechanics of particles. They can apply this knowledge to given problems and solve them. The students can express the new way of thinking in their own words and describe the fundamental differences to classical mechanics. They can also assess which problems are suitable for the application of quantum mechanical methods and what effects the application has on the validity of classical mechanics. Students have gained an overview of the history of quantum mechanics and some fundamental experiments. They are familiar with the content of quantum mechanics and its significance. They have also mastered the necessary mathematical formalism for the representation and computation of quantum theory problems and can apply them.

Content: Mathematical principles and formalism, Schrödinger equation, one-dimensional problems, harmonic oscillators, uncertainty principle, angular momentum, hydrogen atom, potential scattering, density matrix, perturbation theory, basic experiments (e.g. wave-particle duality, diffraction and interference effects, black body radiation, photoelectric effect, Stern-Gerlach experiment)

| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) | |
|--------------------------------------|---|---|-----------------------------------|-------|
| Lecture | 5 | Successful completion of practice tasks | Lecture contact hours | 75 |
| | | | Lecture preparation and follow-up | 60 |
| Practice seminar | 1 | | Prac.S contact hours | 15 |
| | | | Prac.S preparation and follow-up | 30 |
| | | | Written practice tasks | 120 |
| Module examination | none | | | |
| Module language | German | | | |
| Compulsory regular attendance | Attendance recommended | | | |
| Workload, total hours | 300 hours | | | 10 CP |
| Duration of module | One semester | | | |
| Module offered | At least once per academic year | | | |
| Applicability | Master's program Computational Sciences | | | |

2. Scientific Computing area

a) Computer Science

- For the description of the module Complex Algorithms A, see above under 1 Synchronization area, 2 Discipline-related modules, part d) Computer Science

| Module: Complex Algorithms B | | | | |
|--|---|--|-----------------------------------|-------|
| University/Department: Freie Universität Berlin/Mathematics and Computer Science | | | | |
| Responsible for the module: Module lecturers | | | | |
| Admission requirements: none | | | | |
| Qualification objectives: The students have mastered the principles of the current design techniques for algorithms and can use them to design algorithms. They can analyze algorithms in relation to their time and memory requirements, applying advanced analysis methods. They understand the principles of the theory of NP completeness. They know the most common complexity classes and can classify simple problems according to their complexity. They further develop these skills independently in a selected topic area of higher computing science. The students can apply complex algorithms to one of the following topics: distributed systems, pattern recognition, database technology or artificial intelligence. | | | | |
| Content: The module covers aspects of the following topics: path and flow problems in graphs; string matching; randomized algorithms; amortized analysis; the 'master theorem' for the analysis of divide-and-conquer recursion equations; NP completeness; approximation algorithms for difficult problems; number-theoretic algorithms (including RSA cryptosystems); arithmetic algorithms and circuits and Fast Fourier Transform. These topics are subsequently examined in more depth. The following topics may also be covered: | | | | |
| <ul style="list-style-type: none"> - Distributed systems, distributed algorithms, distributed data management, search methods for solving combinatorial tasks - First-order logic and its mechanization, resolution and theorem proofs, knowledge-based and expert systems, fuzzy logic - Bayesian pattern recognition, clustering, expectation maximization, neural networks and learning algorithms, associative networks, recurrent networks. Computer vision with neural networks - Database access technologies and query optimization; realization of transactions, particularly synchronization methods; technological measures to make database systems fault-tolerant. Methods of efficient management of different types of large data sets, in particular of XML documents; correct implementation of transactional guarantees in data management systems | | | | |
| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) | |
| Lecture | 4 | - | Lecture contact hours | 60 |
| | | | Lecture preparation and follow-up | 80 |
| Practice seminar | 2 | - written completion of the work sheets - two oral presentations, each showing the solution of one practice task in the practice seminar | S contact hours | 30 |
| | | | S preparation and follow-up | 60 |
| | | | Prac.S contact hours | 30 |
| | | | Prac.S preparation and follow-up | 60 |
| Seminar | 2 | Preparation and presentation of a research topic | Written practice tasks | 70 |
| | | | Preparation for examination | |
| | | | Examination | |
| Module examination | | Written examination (90 minutes), which may also be carried out as an electronic examination, or oral examination (approx. 30 minutes) or term paper (approx. 15 pages). | | |
| Module language | | German | | |
| Compulsory regular attendance | | Attendance recommended | | |
| Workload, total hours | | 450 hours | | 15 CP |
| Duration of module | | One or two semesters | | |
| Module offered | | At least once per academic year | | |
| Applicability | | Master's program Computational Sciences | | |

- For the description of the module Computer Science and Data Structures A see above under 1. Synchronization area, 2. Discipline-related modules, part d) Computer Science

| Module: Computer Science and Data Structures B | | | | |
|---|---|-------------------------------|------------------|--|
| University/Department: Freie Universität Berlin/Mathematics and Computer Science | | | | |
| Responsible for the module: Module lecturers | | | | |
| Admission requirements: none | | | | |
| Qualification objectives: The students can develop object-oriented software: they can deal with data abstraction, inheritance, and polymorphic type systems and are able to specify and implement abstract data types, to carry out soundness proofs for the implementation of abstract data types, and to take decisions on selecting the most suitable data representation taking efficiency analyses into account. They are familiar with the main abstract data types and their current implementations and the relevant interfaces and classes from the libraries of the programming language used. | | | | |
| Content: The module's starting point is information hiding and its significance for structuring programs and constructing data objects using modules and classes. The term data abstraction, linked with the distinction between specification and implementation of abstract data objects and data types, plays a crucial part in data modeling. Sequences, sets, relations, trees, graphs and geometrical objects are introduced as abstract types. Finally, efficiently manipulable representations of these types are studied and the related algorithms examined for their complexity. | | | | |
| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) | |

| | | | | |
|--------------------------------------|---|--|--|----------------------|
| Lecture | 4 | - | Lecture contact hours Lecture preparation and follow-up | 60 80 |
| Practice seminar | 2 | - written completion of the work sheets - two oral presentations, each showing the solution of one practice task in the practice seminar | S contact hours S preparation and follow-up Prac.S contact hours Prac.S preparation and follow-up | 30 60 30 60 |
| Seminar | 2 | Preparation and presentation of a programming project | Written practice tasks Preparation for examination Examination | 70 |
| Module examination | | Written examination (90 minutes), which may also be carried out as an electronic examination, or oral examination (approx. 30 minutes) or term paper (approx. 15 pages). | | |
| Module language | | German | | |
| Compulsory regular attendance | | Attendance recommended | | |
| Workload, total hours | | 450 hours | | 15 CP |
| Duration of module | | One or two semesters | | |
| Module offered | | At least once per academic year | | |
| Applicability | | Master's program Computational Sciences | | |

- For the description of the module Computer Science and Functional Programming A see above under 1. Synchronization area, 2. Discipline-related modules, part d) Computer Science

| | | | | |
|--|--|--|--|----------------------|
| Module: Computer Science and Functional Programming B | | | | |
| University/Department: Freie Universität Berlin/Mathematics and Computer Science | | | | |
| Responsible for the module: Module lecturers | | | | |
| Admission requirements: none | | | | |
| Qualification objectives: The students are able to functionally design elementary algorithms, to formally specify demands on functional programs, to develop well-structured functional programs, to examine the complexity of functional programs and to formally prove the properties of functional programs. They understand the principles of computability. | | | | |
| Content: Principles of computability (Lambda calculus, primitive recursion, μ -recursion). Introduction to functional programming (syntax, primitive data types, lists, tuples, strings, expressions, function definitions, recursion and iteration, higher order functions, polymorphism, type systems, type inference and type checking, algebraic and abstract data types, input and output, search and sorting algorithms). Proving program properties (rewriting, structural induction, scheduling). Implementation and programming technique (evaluation strategies for functional programs, modular program design). | | | | |
| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) | |
| Lecture | 4 | - | Lecture contact hours Lecture preparation and follow-up | 60 80 |
| Practice seminar | 2 | - written completion of the work sheets - two oral presentations, each showing the solution of one practice task in the practice seminar | S contact hours S preparation and follow-up Prac.S contact hours Prac.S preparation and follow-up | 30 60 30 60 |
| Seminar | 2 | Preparation and presentation of a programming project | Written practice tasks Preparation for examination Examination | 70 |
| Module examination | | Written examination (90 minutes), which may also be carried out as an electronic examination, or oral examination (approx. 30 minutes) or term paper (approx. 15 pages). | | |
| Module language | | German | | |
| Compulsory regular attendance | | Attendance recommended | | |
| Workload, total hours | | 450 hours | | 15 CP |
| Duration of module | | One or two semesters | | |
| Module offered | | At least once per academic year | | |
| Applicability | | Master's program Computational Sciences | | |

- For the description of the module Computer Science and Object-Oriented Programming A see above under 1. Synchronization area, 2. Discipline-related modules, part d) Computer Science

| |
|---|
| Module: Computer Science and Object-oriented Programming B |
|---|

| University/Department: Freie Universität Berlin/Mathematics and Computer Science | | | |
|---|---|--|--|
| Responsible for the module: Module lecturers | | | |
| Admission requirements: none | | | |
| Qualification objectives: The students can specify algorithms in relation to their condition, develop well-structured imperative programs, analyze the complexity of imperative programs and formally prove the properties of imperative programs. | | | |
| Content: Principles of computability (universal register machines, syntax and operational semantics of imperative programming languages); formal methods for specification and verification of imperative programs: (conditions of the state-space, Hoare logic, partial soundness, termination); concepts of imperative and object-oriented programming (primitive and combined data types, methods, parameter passing, overloading, modules, classes, objects, class hierarchies, inheritance, abstract classes, interfaces); programming methodology (incremental correct program development, divide-and-conquer, backtracking, analyzing time and memory requirements, big O notation, transforming recursion into iteration, analyzing search and sorting algorithms). | | | |
| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) |
| Lecture | 4 | - | Lecture contact hours 60 Lecture preparation and follow-up 80 |
| Practice seminar | 2 | - written completion of the work sheets - two oral presentations, each showing the solution of one practice task in the practice seminar | S contact hours 30 S preparation and follow-up 60 Prac.S contact hours 30 Prac.S preparation and follow-up 60 |
| Seminar | 2 | Preparation and presentation of a programming project | Written practice tasks 70 Preparation for examination Examination |
| Module examination | | Written examination (90 minutes), which may also be carried out as an electronic examination, or oral examination (approx. 30 minutes) or term paper (approx. 15 pages). | |
| Module language | | German | |
| Compulsory regular attendance | | Attendance recommended | |
| Workload, total hours | | 450 hours | 15 CP |
| Duration of module | | One or two semesters | |
| Module offered | | At least once per academic year | |
| Applicability | | Master's program Computational Sciences | |

b) Numerics

- For the description of the Introduction to module Numerical Mathematics A see above under I. Synchronization area, 2. Discipline-related modules, part e) Mathematics

| Module: Introduction to Numerical Mathematics B | | | |
|---|---|---|---|
| University/Department: Freie Universität Berlin/ Mathematics and Computer Science | | | |
| Responsible for the module: Module lecturers | | | |
| Admission requirements: none | | | |
| Qualification objectives: The students have mastered advanced numerical solution methods for elementary algebra problems and ordinary differential equations. They have developed a sense for the mathematical structure of these problems and can select and develop reliable and efficient solution algorithms. During the seminars, the students have applied what they have learnt to practical problems of scientific computation and gained an insight into the mathematical modeling of this type of problem. | | | |
| Content: Solution methods for linear equation systems, Cholesky decomposition and QR decomposition, eigenvalue problems, best approximations, polynomial and spline interpolation, Gaussian quadrature and adaptive quadrature. Initial value problems for ordinary differential equations | | | |
| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) |
| Lecture | 4 | - | Lecture contact hours 60 Lecture preparation and follow-up 80 |
| Practice seminar | 2 | Successful completion of practice tasks | S contact hours 30 S preparation and follow-up 60 Prac.S contact hours 30 60 |

| | | | | |
|--------------------------------------|---|--|--|----------|
| Seminar | 2 | Preparation and presentation of a research topic or programming project | Prac.S preparation and follow-up Written practice tasks Preparation for examination Examination | 60 70 |
| Module examination | | Written examination (90 minutes), which may also be carried out as an electronic examination, or oral examination (approx. 30 minutes) or term paper (approx. 15 pages). | | |
| Module language | | German | | |
| Compulsory regular attendance | | Attendance recommended | | |
| Workload, total hours | | 450 hours | | 15 CP |
| Duration of module | | One or two semesters | | |
| Module offered | | At least once per academic year | | |
| Applicability | | Master's program Computational Sciences | | |

- For the description of the module Introduction to Numerics of ODEs and numerical linear algebra A see above under I. Synchronization area, 2. Discipline-related modules, part e) Mathematics

| | | | | |
|--|--|--|--|----------------------|
| Module: Numerics of ODEs and numerical linear algebra B | | | | |
| University/Department: Freie Universität Berlin/ Mathematics and Computer Science | | | | |
| Responsible for the module: Module lecturers | | | | |
| Admission requirements: none | | | | |
| Qualification objectives: The students have in-depth knowledge of numerical solution methods for ordinary differential equations and numerical linear algebra and can deal with them confidently. During the seminars, the students have applied what they have learnt to practical problems of scientific computation and gained an insight into the mathematical modeling of this type of problem. | | | | |
| Content: Selection from the following topics: <ul style="list-style-type: none"> - Initial value problems for stiff differential equations (stability and asymptotic stability of fixed points, test equations) - Implicit Runge-Kutta methods (inheritance methods, stability fields, A- and B-stability, Gaussian method) - Differential algebraic equations (basic terminology, index) - Hamiltonian systems (energy conservation, symplecticism, symplectic Rung-Kutta method) - Iterative methods for solving large linear equation systems (linear iterative methods, preconditioning, method of steepest descent, conjugate gradient method) | | | | |
| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) | |
| Lecture | 4 | - | Lecture contact hours Lecture preparation and follow-up | 60 80 |
| Practice seminar | 2 | Successful completion of practice tasks | S contact hours S preparation and follow-up | 30 60 |
| Seminar | 2 | Preparation and presentation of a research topic or programming project | Prac.S contact hours Prac.S preparation and follow-up Written practice tasks Preparation for examination Examination | 30 60 60 70 |
| Module examination | | Written examination (90 minutes), which may also be carried out as an electronic examination, or oral examination (approx. 30 minutes) or term paper (approx. 15 pages). | | |
| Module language | | German or English | | |
| Compulsory regular attendance | | Attendance recommended | | |
| Workload, total hours | | 450 hours | | 15 CP |
| Duration of module | | One or two semesters | | |
| Module offered | | At least once per academic year | | |
| Applicability | | Master's program Computational Sciences | | |

- For the description of the module Introduction to Numerics of partial differential equations A see above under I. Synchronization area, 2. Discipline-related modules, part e) Mathematics

| | | | | |
|---|--|--|--|--|
| Module: Numerics of partial differential equations B | | | | |
| University/Department: Freie Universität Berlin/ Mathematics and Computer Science | | | | |
| Responsible for the module: Module lecturers | | | | |
| Admission requirements: none | | | | |
| Qualification objectives: The students have in-depth knowledge of numerical solutions for partial differential equations and numerical linear algebra and can deal with them confidently. During the seminars, the students have applied what they have learnt to practical problems of scientific computation and gained an insight into the mathematical modeling of | | | | |

| this type of problem. | | | |
|---|---|--|--|
| Content: Selection from the following topics: | | | |
| <ul style="list-style-type: none"> - Mathematical modeling with partial differential equations - Classification (elliptic, parabolic, hyperbolic) and well-posedness - Classical solutions and finite differences (maximum principle, consistency, convergence) - Weak solutions and finite elements (Sobolev spaces, error estimates, partial volume correction methods) - parabolic differential equations (method of lines, Rothe's method) | | | |
| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) |
| Lecture | 4 | - | Lecture contact hours 60 Lecture preparation and follow-up 80 |
| Practice seminar | 2 | Successful completion of practice tasks | S contact hours 30 S preparation and follow-up 60 |
| Seminar | 2 | Preparation and presentation of a research topic or programming project | Prac.S contact hours 30 Prac.S preparation and follow-up 60 Written practice tasks 60 Preparation for examination 70 Examination |
| Module examination | | Written examination (90 minutes), which may also be carried out as an electronic examination, or oral examination (approx. 30 minutes) or term paper (approx. 15 Pages). | |
| Module language | | German or English | |
| Compulsory regular attendance | | Attendance recommended | |
| Workload, total hours | | 450 hours | 15 CP |
| Duration of module | | One or two semesters | |
| Module offered | | At least once per academic year | |
| Applicability | | Master's program Computational Sciences | |

c) Statistics

- For the description of the module Computational Statistical Physics I A see above under I. Synchronization area, 2. Discipline-related modules, part g) Physics

| Module: Computational Statistical Physics I B | | | |
|---|---|--|--|
| University/Department: Freie Universität Berlin/Physics | | | |
| Responsible for the module: Module lecturers | | | |
| Admission requirements: none | | | |
| Qualification objectives: The students are able to name and describe the principle concepts and theorems of statistical physics and thermodynamics. They are also capable of applying the methods they have learnt to existing problems and to solve them. The students have also mastered the computation methods necessary for dealing with statistical physics and thermodynamics and are able to apply them. They can apply their knowledge of methodology and computation methods in the field of statistical physics to complex issues. | | | |
| Content: Elementary statistics and the laws of large numbers, equilibrium ensembles, the principle of maximum entropy, main theorems of thermodynamics, thermodynamic potentials, thermodynamic processes, phase transition, ideal quantum gases, interactive systems. | | | |
| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) |
| Lecture | 4 | - | Lecture contact hours 60 Lecture preparation and follow-up 80 |
| Practice seminar | 2 | Successful completion of practice tasks | S contact hours 30 S preparation and follow-up 60 |
| Seminar | 2 | Preparation and presentation of a research topic or programming project | Prac.S contact hours 30 Prac.S preparation and follow-up 60 Written practice tasks 60 Preparation for examination 70 Examination |
| Module examination | | Written examination (90 minutes), which may also be carried out as an electronic examination, or oral examination (approx. 30 minutes) or term paper (approx. 15 pages). | |

| | | |
|--------------------------------------|---|-------|
| Module language | English | |
| Compulsory regular attendance | Attendance recommended | |
| Workload, total hours | 450 hours | 15 CP |
| Duration of module | One or two semesters | |
| Module offered | At least once per academic year | |
| Applicability | Master's program Computational Sciences | |

- For the description of the module Computational Statistical Physics II A see above under I. Synchronization area, 2. Discipline-related modules, part g) Physics

| Module: Computational Statistical Physics II B | | | | |
|---|--|--|-----------------------------------|----|
| University/Department: Freie Universität Berlin/Physics | | | | |
| Responsible for the module: Module lecturers | | | | |
| Admission requirements: none | | | | |
| Qualification objectives: The students have in-depth knowledge of the fundamental concepts and theorems of statistical physics. They can name, describe and apply them and apply the methods they have learnt to given problems to solve them. The students have extended their knowledge of methods and calculation methods in the field of statistical physics and are now able to apply these to complex issues. Using the methods they have learnt, they are also able to derive and analyze microscopic physical processes / laws at the macroscopic level. | | | | |
| Content: A selection of the following advanced topics of statistical physics: non-equilibrium thermodynamics (entropy production, Onsager relations), linear response theory and fluctuation-dissipation theorem, stochastic processes (Markov processes, master equation, Langevin equation and Fokker-Planck equation), kinetic theory, phase transitions (Landau theory, Gaussian fluctuations, correlation functions, renormalization groups), theory of liquids, hydrodynamics and elasticity, statistical quantum mechanics, exactly solvable models. | | | | |
| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) | |
| Lecture | 4 | - | Lecture contact hours | 60 |
| | | | Lecture preparation and follow-up | 80 |
| Practice seminar | 2 | Successful completion of practice tasks | S contact hours | 30 |
| | | | S preparation and follow-up | 60 |
| Seminar | 2 | Preparation and presentation of a research topic or programming project | Prac.S contact hours | 30 |
| | | | Prac.S preparation and follow-up | 60 |
| | | | Written practice tasks | 70 |
| | | | Preparation for examination | |
| | | | Examination | |
| Module examination | | Written examination (90 minutes), which may also be carried out as an electronic examination, or oral examination (approx. 30 minutes) or term paper (approx. 15 pages). | | |
| Module language | | English | | |
| Compulsory regular attendance | | Attendance recommended | | |
| Workload, total hours | | 450 hours | 15 CP | |
| Duration of module | | One or two semesters | | |
| Module offered | | At least once per academic year | | |
| Applicability | | Master's program Computational Sciences | | |

III. Specialization area

1. Molecular Sciences

a) Required modules:

| Module: Molecular Simulation I | | | | |
|---|---|--|-----------------------------------|----|
| University/Department: Freie Universität Berlin/Mathematics and Computer Science, Physics | | | | |
| Responsible for the module: Module lecturers | | | | |
| Admission requirements: none | | | | |
| Qualification objectives: The students learn the theoretical principles and simulation techniques for simple stochastic systems (e.g. molecule models, Ising models, diffusion in model potentials). They understand the physical principles and relations between stochastic trajectories and ensembles, can generate simulation data and estimate expectation values. They can apply what they have learnt confidently. | | | | |
| Content: <i>Thermostatistics:</i> Principles and derivations for the most important ensembles. Boltzmann distribution, partition functions, expectation values <ul style="list-style-type: none"> - <i>Monte-Carlo method:</i> Theory, construction, convergence and implementation of the Monte-Carlo method for calculating stationary expectation values - <i>Kinetics:</i> Theory of rates, time correlations and other time-dependent expectation values - <i>Molecular dynamic simulation:</i> Theory, construction, convergence and implementation of molecular dynamic simulations to calculate time-dependent expectation values This module complements Molecular Simulation II. We recommend taking first Molecular Simulation I followed by Molecular Simulation II, but this is not strictly necessary. | | | | |
| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) | |
| Lecture | 2 | - | Lecture contact hours | 30 |
| | | | Lecture preparation and follow-up | 30 |
| Practice seminar | 2 | Successful completion of practice worksheets and oral presentation of solutions | Prac.S contact hours | 30 |
| | | | Prac.S preparation and follow-up | 30 |
| | | | Preparation for examination | 30 |
| | | | Examination | |
| Module examination | | Written examination (90 minutes), which may also be carried out as an electronic examination, or oral examination (approx. 30 minutes) or term paper (approx. 15 pages). | | |
| Module language | | English | | |
| Compulsory regular attendance | | Attendance recommended | | |
| Workload, total hours | | 150 hours | 5 CP | |
| Duration of module | | One semester | | |
| Module offered | | At least once per academic year | | |
| Applicability | | Master's program Computational Sciences | | |

For the module Quantum Chemistry (5 CP) you are referred to the study and examination regulations for the Master's program Chemistry of the Department Biology, Chemistry, Pharmacy at the Freie Universität Berlin.

b) Compulsory elective modules:

For the module Density Functional Theory (5 CP) you are referred to the study and examination regulations for the Master's program Chemistry of the Department Biology, Chemistry, Pharmacy at the Freie Universität Berlin.

| Module: Research Project A | | | | |
|--|---|-------------------------------|------------------|--|
| University/Department: Freie Universität Berlin/Biology, Chemistry, Pharmacy/Earth Sciences/ Mathematics and Computer Science/Physics | | | | |
| Responsible for the module: Module lecturers | | | | |
| Admission requirements: none | | | | |
| Qualification objectives: The students can apply their knowledge, skills and abilities in scientific computing in a current research project, as far as possible industry-related. They can work in teams and communicate appropriately about their work. They are willing to offer assistance within the team if necessary; they can select and evaluate the appropriate aids and offer factual criticism. | | | | |
| Content: In this module, the students work on application-oriented problems supported by scientific computing methods. | | | | |
| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) | |

| | | | | |
|--------------------------------------|---|--|------------------------------|-----|
| Project seminar | 2 | Contributions to discussion | PS contact hours | 30 |
| | | | PS preparation and follow-up | 100 |
| | | | Preparation for examination | |
| | | | Examination | 20 |
| Module examination | | Lecture (approx. 15 minutes) with written paper on the student's individual project contribution (approx. 5 pages) | | |
| Module language | | English | | |
| Compulsory regular attendance | | Attendance recommended | | |
| Workload, total hours | | 150 hours | 5 CP | |
| Duration of module | | One semester | | |
| Module offered | | At least once per academic year | | |
| Applicability | | Master's program Scientific Computing | | |

| | | | | |
|--|--|---|------------------------------|-----|
| Module: Research project E | | | | |
| University/Department: Freie Universität Berlin/Biology, Chemistry, Pharmacy / Earth Sciences / Mathematics and Computer Science / Physics | | | | |
| Responsible for the module: Module lecturers | | | | |
| Admission requirements: none | | | | |
| Qualification objectives: The students can apply their knowledge, skills and abilities in scientific computing in a current research project, as far as possible industry-related. They can work in teams and communicate appropriately about their work. They are willing to offer assistance within the team if necessary; they can select and evaluate the appropriate aids and offer factual criticism. | | | | |
| Content: In this module, the students work on application-oriented problems supported by scientific computing methods. | | | | |
| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) | |
| Project seminar | 4 | Regular contributions to discussion | PS contact hours | 60 |
| | | | PS preparation and follow-up | 210 |
| | | | Preparation for examination | |
| | | | Examination | 30 |
| Module examination | | Lecture (approx. 30 minutes) with written paper on the student's individual project contribution (approx. 10 pages) | | |
| Module language | | English | | |
| Compulsory regular attendance | | Attendance recommended | | |
| Workload, total hours | | 300 hours | 10 CP | |
| Duration of module | | One semester | | |
| Module offered | | At least once per academic year | | |
| Applicability | | Master's program Scientific Computing | | |

| | | | | |
|---|--|---|-----------------------------|----|
| Module: Research Seminar Computational Sciences | | | | |
| University/Department: Freie Universität Berlin/Biology, Chemistry, Pharmacy / Earth Sciences / Mathematics and Computer Science / Physics | | | | |
| Responsible for the module: Module lecturers | | | | |
| Admission requirements: none | | | | |
| Qualification objectives: The students can work independently to familiarize themselves with current topics by reading specialist literature, prepare a topic for presentation and acquire supplementary background information. They can present even difficult topics in comprehensible form in lectures. They can highlight essential elements among less important elements and pay particular attention to the selection of appropriate media. They are willing to ask questions when an issues is unclear; they can take part in discussions on scientific issues and offer factual criticism. | | | | |
| Content: Current research topics are examined in this seminar, giving students the opportunity to prepare themselves for their Master's thesis. | | | | |
| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) | |
| Seminar | 2 | Regular contributions to discussion | S contact hours | 30 |
| | | | S preparation and follow-up | 30 |
| | | | Preparation for examination | |
| | | | Examination | 90 |
| Module examination | | Presentation of a research project or a topic from specialist literature (approx. 45 minutes) | | |
| Module language | | English | | |

| | | |
|--------------------------------------|---------------------------------------|------|
| Compulsory regular attendance | Attendance recommended | |
| Workload, total hours | 150 hours | 5 CP |
| Duration of module | One semester | |
| Module offered | Not offered regularly | |
| Applicability | Master's program Scientific Computing | |

| | | | | |
|---|--|--|--|--------------------|
| Module: Markov modeling | | | | |
| University/Department: Freie Universität Berlin/Mathematics and Computer Science | | | | |
| Responsible for the module: Module lecturers | | | | |
| Admission requirements: none | | | | |
| Qualification objectives: The students learn the theoretical principles of conformational dynamics and the discrete description of continuous-state-space Markov processes. They can apply what they have learnt confidently using selected numerical and computer-supported methods. They are willing to ask questions when an issue is unclear; they can take part in discussions on scientific issues and offer factual criticism. | | | | |
| Content: | | | | |
| <ul style="list-style-type: none"> - <i>Markov chains:</i> Theory on space-time-discrete Markov chains. Irreducibility, ergodicity, reversibility. Algorithms for calculating these properties. - <i>Model estimation and error estimation:</i> Methods for estimation of reversible and non-reversible models. Bayes theorem. Sampling method for estimating reversible and non-reversible models. Linear error perturbation - <i>Simulation and convergence:</i> Convergence of estimated values and improving the convergence - <i>Ensemble analysis:</i> Eigenvalues and eigenvectors of the transition matrix; correlation functions. Measurement values for molecular experiments - <i>Trajectory analysis:</i> Mean first passage times, committor functions, transition path theory - <i>Discretization:</i> Approximation of continuous Markov processes by Markov chains. Approximation errors. Variational principle | | | | |
| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) | |
| Lecture | 2 | - | Lecture contact hours Lecture preparation and follow-up | 30 30 |
| Practice seminar | 2 | Successful completion of practice worksheets and oral presentation of solutions | Prac.S contact hours Prac.S preparation and follow-up Preparation for examination Examination | 30 30 30 |
| Module examination | | Written examination (90 minutes), which may also be carried out as an electronic examination, or oral examination (approx. 30 minutes) or term paper (approx. 15 pages). | | |
| Module language | | English | | |
| Compulsory regular attendance | | Attendance recommended | | |
| Workload, total hours | | 150 hours | 5 CP | |
| Duration of module | | One semester | | |
| Module offered | | At least once per academic year | | |
| Applicability | | Master's program Computational Sciences | | |

| | | | | |
|---|--|--------------------------------------|----------------------------|--|
| Module: Molecular simulation II | | | | |
| University/Department: Freie Universität Berlin/ Mathematics and Computer Science, Physics | | | | |
| Responsible for the module: Module lecturers | | | | |
| Admission requirements: none | | | | |
| Qualification objectives: The students learn classical (not quantum-mechanical) models for molecules, in particular macromolecules and biomolecules. They can apply what they have learnt confidently. | | | | |
| Content: | | | | |
| <ul style="list-style-type: none"> • <i>Energy function:</i> Structure, importance and parametrization of empirical energy functions in classical molecular dynamics • <i>Algorithms and data structures:</i> Periodic boundary conditions, cut-off, efficient neighbor search • <i>Long-range interactions:</i> Coulomb summation, convergence, Poisson's equation, Ewald summation, Particle Mesh methods • <i>Solvation methods:</i> Explicit, Poisson-Boltzmann, Generalized Born • <i>Dynamics:</i> Integrators, discretization errors • <i>Sampling methods:</i> Metastability, replica exchange, umbrella sampling • <i>Expectation values:</i> Calculating expectation values from molecular simulations <p>This module complements Molecular Simulation I. We recommend taking first Molecular Simulation I followed by Molecular Simulation II, but this is not strictly necessary. Practical skills are taught in a simulation practical. This is usually a block unit and takes place in the lecture-free phase.</p> | | | | |
| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) | |

| | | | | |
|--------------------------------------|---|--|--|--------------------|
| Lecture | 2 | Active participation and discussion | Lecture contact hours Lecture preparation and follow-up | 30 30 |
| Practice seminar (Block) | 2 | Successful completion of simulation and programming tasks | Prac.S contact hours Prac.S preparation and follow-up Preparation for examination Examination | 30 30 30 |
| Module examination | | Written examination (90 minutes), which may also be carried out as an electronic examination, or oral examination (approx. 30 minutes) or term paper (approx. 15 pages). | | |
| Module language | | English | | |
| Compulsory regular attendance | | Attendance recommended | | |
| Workload, total hours | | 150 hours | 5 CP | |
| Duration of module | | One semester / block | | |
| Module offered | | Not offered regularly | | |
| Applicability | | Master's program Computational Sciences | | |

For the modules Quantum Correlation Methods (5 CP) and Quantum Reaction Dynamics (5CP), you are referred to the study and examination regulations for the Master's program Chemistry of the Department Biology, Chemistry, Pharmacy at the Freie Universität Berlin.

| | | | | |
|---|--|--|--|--------------------|
| Module: Selected topics in theoretical computational sciences | | | | |
| University/Department: Freie Universität Berlin/Biology, Chemistry, Pharmacy/Earth Sciences/ Mathematics and Computer Science/Physics | | | | |
| Responsible for the module: Module lecturers | | | | |
| Admission requirements: none | | | | |
| Qualification objectives: The students know the principles of a selected research field in scientific computing and understand the relevant terminology. They can apply what they have learnt confidently. They are willing to ask questions when an issue is unclear; they can participate in discussions on scientific issues and offer factual criticism. | | | | |
| Content: The module gives an introduction to a selected research area of scientific computing. Current research issues are also examined. | | | | |
| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) | |
| Lecture | 2 | - | Lecture contact hours Lecture preparation and follow-up | 30 30 |
| Practice seminar | 2 | Successful completion of practice worksheets and oral presentation of solutions | Prac.S contact hours Prac.S preparation and follow-up Preparation for examination Examination | 30 30 30 |
| Module examination | | Written examination (90 minutes), which may also be carried out as an electronic examination, or oral examination (approx. 30 minutes) or term paper (approx. 15 pages). | | |
| Module language | | English | | |
| Compulsory regular attendance | | Practice seminar: yes; Lecture: Attendance recommended | | |
| Workload, total hours | | 150 hours | 5 CP | |
| Duration of module | | One semester | | |
| Module offered | | Not offered regularly | | |
| Applicability | | Master's program Scientific Computing | | |

| | | | | |
|---|--|--------------------------------------|----------------------------|--|
| Module: Selected topics in applied computational sciences | | | | |
| University/Department: Freie Universität Berlin/Biology, Chemistry, Pharmacy/Earth Sciences/ Mathematics and Computer Science/Physics | | | | |
| Responsible for the module: Module lecturers | | | | |
| Admission requirements: none | | | | |
| Qualification objectives: The students know the principles of a selected field in scientific computing and can work independently to develop solutions to selected problems. They are willing to ask questions when an issue is unclear; they can participate in discussions on scientific issues and offer factual criticism. | | | | |
| Content: The module gives insight into a selected area of scientific computing. Current research issues and areas of application are also examined. | | | | |
| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) | |

| | | | | |
|--------------------------------------|---|--|--|--------------------|
| Lecture | 2 | Active participation and where applicable, discussion | Lecture contact hours Lecture preparation and follow-up | 30 30 |
| Seminar on the computer | 1 | Successful completion of computer practice tasks | SPC contact hours SPC preparation and follow-up Preparation for examination Examination | 15 15 60 |
| Module examination | | Written examination (90 minutes), which may also be carried out as an electronic examination, or oral examination (approx. 30 minutes) or term paper (approx. 15 pages). | | |
| Module language | | English | | |
| Compulsory regular attendance | | Attendance recommended | | |
| Workload, total hours | | 150 hours | 5 CP | |
| Duration of module | | One semester | | |
| Module offered | | Not offered regularly | | |
| Applicability | | Master's program Scientific Computing | | |

2. Geosciences

a) Required modules :

For the modules Geophysics I (6 CP) and Seismics II (6 CP), students are referred to the Study and Examination Regulations for the Master's program Geological Sciences of the Department of Earth Sciences at the Freie Universität Berlin.

b) Compulsory elective modules:

For the module Earth Dynamics (6 CP), students are referred to the Study and Examination Regulations for the Master's program Geological Sciences of the Department of Earth Sciences at the Freie Universität Berlin.

| | | | | |
|--|--|--|--|---------------------|
| Module: Research Project C | | | | |
| University/Department: Freie Universität Berlin/Biology, Chemistry, Pharmac / Earth Sciences / Mathematics and Computer Science / Physics | | | | |
| Responsible for the module: Module lecturers | | | | |
| Admission requirements: none | | | | |
| Qualification objectives: The students can apply their knowledge, skills and abilities in scientific computing in a current research project, as far as possible industry-related. They can work in teams and communicate appropriately about their work. They are willing to offer assistance within the team if necessary; they can select and evaluate the appropriate aids and offer factual criticism. | | | | |
| Content: In this module, the students work on application-oriented problems supported by scientific computing methods. | | | | |
| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) | |
| Project seminar | 2 | Regular contributions to discussion | PS contact hours PS preparation and follow-up Preparation for examination Examination | 30 120 60 |
| Module examination | | Lecture (approx. 15 minutes) with written paper on the student's individual project contribution (approx. 5 pages) | | |
| Module language | | English | | |
| Compulsory regular attendance | | Attendance recommended | | |
| Workload, total hours | | 210 hours | 7 CP | |
| Duration of module | | One semester | | |
| Module offered | | At least once per academic year | | |
| Applicability | | Master's program Scientific Computing | | |

For the description of the module Research Seminar Computational Sciences (5 CP) see above under III. Specialization area, 1. Molecular Sciences, part b) compulsory elective modules.

For the description of the module Research Project A (5 CP), see above under III. Specialization area, 1. Molecular Sciences, part b) compulsory elective modules.

For the description of the module Geophysics II (6 CP), students are referred to the Study and Examination Regulations for the Master's program Geological Sciences of the Department of Earth Sciences at the Freie Universität Berlin.

For the description of the modules: Selected topics in theoretical computational sciences (5 CP) und Selected topics in applied computational sciences (5 CP) see above under III. Specialization area, 1. Molecular Sciences, part b) compulsory elective modules.

For the module Thermodynamics und Kinetics of Geological Processes (6 CP), students are referred to the Study and Examination Regulations for the Master's program Geological Sciences of the Department of Earth Sciences at the Freie Universität Berlin.

3. Atmospheric Sciences

a) Required modules:

For the module Weather and Climate Diagnosis (6 CP), students are referred to the Study and Examination Regulations for the Master's program Meteorology of the Department of Earth Sciences at the Freie Universität Berlin.

b) Compulsory elective modules:

| Module: Research project B | | | |
|--|---|--|--|
| University/Department: Freie Universität Berlin/Biology, Chemistry, Pharmacy/Earth Sciences/ Mathematics and Computer Science/Physics | | | |
| Responsible for the module: Module lecturers | | | |
| Admission requirements: none | | | |
| Qualification objectives: The students can apply their knowledge, skills and abilities in scientific computing in a current research project, as far as possible industry-related. They can work in teams and communicate appropriately about their work. They are willing to offer assistance within the team if necessary; they can select and evaluate the appropriate aids and offer factual criticism. | | | |
| Content: In this module, the students work on application-oriented problems supported by scientific computing methods. | | | |
| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) |
| Project seminar | 2 | Regular contributions to discussion | PS contact hours PS preparation and follow-up Preparation for examination Examination |
| | | | 30 130 20 |
| Module examination | | Lecture (approx. 15 minutes) with written paper on the student's individual project contribution (approx. 5 pages) | |
| Module language | | English | |
| Compulsory regular attendance | | Attendance recommended | |
| Workload, total hours | | 180 hours | 6 CP |
| Duration of module | | One semester | |
| Module offered | | At least once per academic year | |
| Applicability | | Master's program Scientific Computing | |

| Supplementary module: Research project D | | | |
|--|---|--|--|
| University/Department: Freie Universität Berlin/ Biology, Chemistry, Pharmacy / Earth Sciences / Mathematics and Computer Science / Physics | | | |
| Responsible for the module: Module lecturers | | | |
| Admission requirements: none | | | |
| Qualification objectives: The students can apply their knowledge, skills and abilities in scientific computing in a current research project, as far as possible industry-related. They can work in teams and communicate appropriately about their work. They are willing to offer assistance within the team if necessary; they can select and evaluate the appropriate aids and offer factual criticism. | | | |
| Content: In this module, the students work on application-oriented problems supported by scientific computing methods. | | | |
| Teaching and learning units | Contact hours (Semester hours per week = SH) | Forms of active participation | Workload (hours) |
| Project seminar | 4 | Regular contributions to discussion | PS contact hours PS preparation and follow-up Preparation for examination Examination |
| | | | 60 180 30 |
| Module examination | | Lecture (approx. 20 minutes) with written paper on the student's individual project contribution (approx. 5 pages) | |
| Module language | | English | |
| Compulsory regular attendance | | Attendance recommended | |
| Workload, total hours | | 270 hours | 9 CP |
| Duration of module | | One semester | |
| Module offered | | At least once per academic year | |
| Applicability | | Master's program Scientific Computing | |

For the description of the module Research Seminar computational sciences (5 CP) see above under III. Specialization area, 1. Molecular Sciences, part b) compulsory elective modules.

For the modules Climate Variability and Climate Models (8 CP), Models for Weather and the Environment (8 CP), and Satellite Meteorology (8 CP), students are referred to the Study and Examination Regulations for the Master's program Meteorology of the Department of Earth Sciences at the Freie Universität Berlin.

For the description of the modules Selected topics in theoretical computational sciences (5 CP) und Selected topics in applied computational sciences (5 CP) see above under III. Specialization area, 1. Molecular Sciences, part b) compulsory elective modules.

For the modules Theoretical Meteorology I (8 CP) and Theoretical Meteorology II (8 CP), students are referred to the Study and Examination Regulations for the Master's program Meteorology of the Department of Earth Sciences at the Freie Universität Berlin.

Annex 2: Sample program schedule

Variant A

| 1st Semester | 2nd Semester | 3rd Semester | 4th Semester |
|--|---|------------------------------|---|
| Synchronization area Required Module Computational Sciences (15 CP) | Scientific Computing area Module A (15 CP) | Specialization area 30 CP | Master's thesis with accompanying colloquium 30 CP |
| Synchronization area Elective module/s totaling 15 CP | Scientific Computing area Module B (15 CP) | | |
| Total: 30 CP | Total: 30 CP | Total: 30 CP | Total: 30 CP |

Variant B

| 1st Semester | 2nd Semester | 3rd Semester | 4th Semester |
|--|---|------------------------------|---|
| Synchronization area Required Module Computational Sciences (15 CP) | Scientific Computing area Module A (15 CP) | Specialization area 30 CP | Master's thesis with accompanying colloquium 30 CP |
| Scientific Computing area Module B (15 CP) | | | |
| Synchronization area Elective module/s totaling 15 CP | | | |
| Total: 30 CP | Total: 30 CP | Total: 30 CP | Total: 30 CP |



Joint Commission
of the Departments Biology, Chemistry, Pharmacy, Earth Sciences,
Mathematics and Computer Science, and Physics at the Freie Universität
Berlin

Certificate of Academic Record

Ms/Mr [first name/surname]

born on [day/month/year] in [place of birth]

has successfully completed the Master's program

Computational Sciences

in accordance with the examination regulations of [day/month/year] (FU-Mitteilungen No. [XX]/year) with the final grade

[Grade as number and text]

and has proved the attainment of the required 120 credit points.

The examination attainments were graded as follows:

| Areas of study | Credit points | Grade |
|---------------------------|---------------|-------|
| Synchronization area | 30 (15) | n.n |
| Scientific Computing area | 30 (15) | n.n |
| Specialization area [XX] | 30 (30) | n.n |
| Master's thesis | 30 (30) | n.n |

The topic of the Master's thesis was: [XX]

Berlin, [day/month/year]

(seal)

Chair of the
Joint Commission

Chair of the
Examination committee

Grade scale: 1.0 – 1.5 very good; 1.6 – 2.5 good; 2.6 – 3.5 satisfactory; 3.6 – 4.0 sufficient; 4.1 – 5.0 insufficient

Evaluation without grades: P – passed; NP – not passed

The credit points comply with the European Credit Transfer and Accumulation System (ECTS).

Not all achievements are graded; the credit points listed in brackets denote the total attainments evaluated with a grade that are taken into consideration in the final grade.

Annex 4: Degree certificate



(sample)

Joint Commission
of the Departments Biology, Chemistry, Pharmacy, Earth Sciences,
Mathematics and Computer Science, and Physics at the Freie Universität
Berlin

Degree Certificate

Ms/Mr [first name/surname]

born on [day/month/year] in [place of birth]

has successfully completed the Master's program in

Computational Sciences

In accordance with the examination regulations of [day/month/year] (FU-Mitteilungen No. [XX]/year)

the university degree of

Master of Science (M. Sc.)

is hereby awarded.

Berlin, [day/month/year]

(Seal)

Chair of the

Joint Commission

Chair of the

Examination Committee